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DIFFERENTIAL CROSS SECTION FOR ELECTRON DETACHMENT FROM NEGATIVE HYDROGEN IONS COLLIDING WITH NEUTRAL HYDROGEN ATOMS.

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DIFFERENTIAL CROSS SECTION FOR ELECTRON

DETACHMENT FROM NEGATIVE HYDROGEN IONS

COLLIDING WITH NEUTRAL HYDROGEN ATOMS

THESIS

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Preface

I would like to extend my sincere appreciation to several people for their assistance in this research. First, I would like to thank my advisor, Dr. Donn Shankland, for his guidance, advice and time that he gave me during this work. I would also like to thank Major Thomas Genoni and Captain Larry Wright of the Nuclear Technology Office, Kirtland Air Force Base, New Mexico for their help in this study. I wish to thank Sherry Markiewicz for her help in typing and finishing this thesis. I extend my sincere thanks to the CDC 6613 and the Cyber 74 for the endless hours of frustration they provided me. Lastly, I would like to thank my wife, Kathy, for providing help, encouragement and, when needed, a shoulder to cry on.

Mark Franz

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Abstract

The first Born Approximation is used to calculate the differential cross section for electron detachment from H^- ions colliding with hydrogen atoms. The differential and total cross sections are evaluated for the resultant hydrogen atom in the 1s or 2s state and the target hydrogen atom in any ecited state up to n = 8. The scattering matrix includes the exchange of particles interaction, which has not been included in earlier work. The results are presented and compared with earlier work where possible.

DIFFERENTIAL CROSS SECTION FOR ELECTRON
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I. Introduction

Background and Previous Work

The recent interest in neutral particle beams has made it necessary for investigators to better understand the theoretical and experimental processes in the production of such beams. There are two basic processes that can be used to create a beam of neutral particles. The first method is to pass a beam of positively charged ions through a gas pick-up cell, where the ions pick-up an electron. The resulting beam consists of neutral particles. The second process is to pass a beam of negatively charged ions through a gas stripping cell, stripping the extra electron from the particles in the beam. The stripping or pick-up reaction has deflected the outgoing beam of particles because of a change of energy and hence there is a momentum transfer. The stripping reaction would deflect the beam less because of the smaller change in energy of the atomic systems as compared to the pick-up reaction. Using the stripping reaction a beam of neutral hydrogen could be produced by stripping an electron from a negatively charged hydrogen ion (H⁻) in a collision with hydrogen or a heavier atomic system.

There are many theoretical questions concerning the process of electron detachment. What is the differential cross section for different energies? What effect do better wavefunctions have on the theoretical differential cross section? How important is exchange? Some of these questions have been answered in the literature. The basic

theoretical concepts for electron detachment were presented by Bates and Griffing (Ref 2 and 3), however their work dealt with finding the total cross section. Sida (Ref 17) calculated the total cross section for electron detachment of H^- ions with helium atoms. The process of H^- ions colliding with H atoms was done by McDowell and Peach (Ref 15). In both cases simple two parameter wave functions were used and no exchange of particles was discussed.

Recently there has been a greater interest in obtaining the differential cross section because it shows explicitly the deflection of the beam from its original direction. Lee and Chen (Ref 13) have calculated the differential cross section for electron detachment from H^- ions in collisions with H atoms using a sum rule technique and summing over all the excited states of the resultant H atom. Genoni and Wright (Ref 8) have also calculated the differential cross section for this process. Their calculations were for the target H atom in final state $N = 1$ to 8 or in a continuous state and the resultant H atom in the 1s or 2s state. Exchange of particles was neglected in both cases.

Purpose and Scope

The purpose of this thesis is to calculate the differential cross section for electron detachment from H^- ions colliding with H atoms. The differential cross section is evaluated using the first term of the Born Series. The H^- ion is initially in its ground state configuration and has a kinetic energy of 1 to 500 MeV in the laboratory frame, while the target hydrogen atom is in its ground state configuration and stationary in the laboratory frame. After the collision the resultant H atom is in the 1s or 2s configuration while the H target atom is in the $N = 1$ to 8 state. The differential cross section and total cross section

is evaluated explicitly for energies of 2 MeV and 200 MeV for the H^- ion.

Units

All quantities in this study are presented in atomic units, where

$$\hbar = m = e = 1$$

and are dimensionless. The speed of light is the inverse of the fine structure constant, α. Length and momenta are also dimensionless while energy is in units of hartrees, where 1 hartree = 27.21 eV. All cross sections are presented in units of πa_o^2 where a_o is a Bohr radius.

General approach

The general approach in the evaluation of the differential and total cross section follows the pattern set in solving any quantum mechanical problem. The general kinematics are discussed with a special emphasis on the relativistic treatment of the scattering problem. The total Hamiltonian is formulated for the system of particles and from the total Hamiltonian the scattering potential, initial and final wavefunction for the particles are found. The scattering matrix can be evaluated using the scattering potential and wavefunctions. Using this scattering matrix, the differential and total cross section are obtained using numerical integration techniques.

II. Formulation of Scattering Problem

In this chapter the basic scattering problem is discussed and explained. An overview of the scattering is presented with special detail given to the energy and momentum considerations. The differential cross section for the final three body problem is derived using Fermis' Golden Rule. Finally a discussion of the Born Series is given and it is shown that only the first term of the Born Series needs to be retained in the calculation of the scattering matrix.

Overview of the Scattering Problem

The scattering problem in general is that of an incoming H^- ion, with energy T, traveling toward a stationary H target atom. After the collision there are three particles in the final state, a free electron and two hydrogen atoms. The resultant H atom (H^- stripped of one electron) has been deflected through some scattering angle θ. The differential cross section associated with the scattering angle θ is to be calculated.

The differential cross section can be evaluated in the laboratory frame, but it is easier to perform the calculations in the center of mass frame and then transform back to the laboratory frame. Therefore in the center of mass frame the H^- ion has momentum

$$\overline{k}_- = \frac{M_o}{M_o + M_-} \overline{k}_i \tag{1}$$

where M_o is the mass of the neutral H atom, M_- is the mass of the H^- ion and $\overline{k}_i$ is the initial momentum of the H^- ion in the laboratory frame. When relativistic effects are included $\overline{k}_i$ is given by

$$\overline{k}_i = \frac{1}{c}\sqrt{T^2 + 2TM_-c^2} \ \hat{v}_i \tag{2}$$

Where T is the incoming energy and $\hat{v}_i$ is the unit vector of the initial velocity. This equation is valid for all incoming energies that need to be considered. In the center of mass frame the H target atom has momentum

$$\overline{k}_o = - \overline{k}_- \tag{3}$$

The total energy of the initial system, in the center of mass frame, is

$$E_a = \frac{k_-^2}{2M_-} + \frac{k_o^2}{2M_o} + E_{H^-}(1s^2) + E_H(1s) \tag{4}$$

where $E_{H^-}(1s^2)$ is the energy bound in the H^- ion system and $E_H(1s)$ is the energy bound in the H target atom system. $E_H(1s)$ is given to be

$$E_H(1s) = -0.5 \text{ a.u.} \tag{5}$$

and from Caveline, et al. (Ref 6:625),

$$E_{H^-}(1s^2) = -0.527751 \text{ a.u.} \tag{6}$$

Using Equation 3, Equation 4 can be rewritten as

$$E_a = \frac{k_-^2}{2\mu_{-o}} + E_H(1s) + E_{H^-}(1s^2) \tag{7}$$

where μ_{-o} is the reduced mass of the H^- ion and H target atom.

The final configuration consists of three particles, a free electron with momentum $\overline{k}_e$, a recoiling target atom with momentum $\overline{k}$ and a resulting H atom with momentum $\overline{k}_H$. From the conservation of momentum argument, the momentum of the H target atom is

$$\overline{k} = - (\overline{k}_H + \overline{k}_e) \tag{8}$$

The total energy of the final system is then

$$E_b = \frac{k_H^2}{2M_o} + \frac{k^2}{2M_o} + \frac{k_e^2}{2m_e} + E_H(nl) + E_H(N) + I_{H^-} \tag{9}$$

where $E_H(nl)$ is the energy bound in the resultant H atom when $nl = 1s$

or 2s, E_H (N) is the energy bound in the target atom when its final

state is N = 1 to 8 and I_{H^-} is the ionization energy of the H^- ion,

from Ref 6,

$$I_{H^-} = 0.76 \text{ eV} = 2.793 \times 10^{-2} \text{ a.u.} \tag{10}$$

Using Equation 8, Equation 9 can be rewritten as

$$E_b = \frac{k_H^2}{2M_o} + \frac{k_e^2}{2\mu_{oe}} + \frac{2\overline{k}_e \cdot \overline{k}_H}{2M_o} + E_H (N) + E_H (nl) + I_{H^-} \tag{11}$$

where μ_{oe} is the reduced mass of a hydrogen atom and an electron.

The conservation of energy requires that

$$E_a = E_b \tag{12}$$

or

$$\frac{k_-^2}{2\mu} + E_{H^-} (1s^2) + E_H (1s) =$$

$$\frac{k_H^2}{M_o} + \frac{k_e^2}{2\mu_{oe}} + \frac{2\overline{k}_i \overline{k}_H}{2m} + E_H (N) + E_H (nl) + I_{H^-} \tag{13}$$

Denoting

$$E_f = \frac{k_-^2}{2\mu} + E_{H^-} (1s^2) + E_H (1s) - E_H (nl) - E_H (N) - I_{H^-} \tag{14}$$

$$= \frac{k_-^2}{2\mu} - 1.0 \text{ a.u.} + .5 \left[\frac{1}{n^2} + \frac{1}{N^2} \right] \text{ a.u.} \tag{15}$$

allows Equation 13 to be written as

$$E_f = \frac{k_H^2}{M_o} + \frac{k_e^2}{2\mu_{eo}} + \frac{2\overline{k}_e \cdot \overline{k}_H}{2M_o} \tag{16}$$

The term on the right represents all the known quantities while the

terms on the left represents the unknowns $\overline{k}_H$ and $\overline{k}_e$.

Formulation of Differential Cross Section With Three Final Particles

The scattering of one particle with another can be treated as a

time-dependent perturbation where the potential is "turned on" when

the incident particle is in the vicinity of the target particle, and

then the potential is "turned off" as the particles leave the vicinity of each other. The scattering process can be considered as a time-dependent transition from an initial wave state, $|i\rangle$ to a final wave state, $|f\rangle$. For the problem under consideration, the initial wave state consists of the wave functions for the H target atom and the H^- ion. The final wave function consists of the wave functions for the H target atom, the resultant H atom and the free electron. The transition rate per incident particle is given by Fermis' Golden Rule

$$R = \frac{2\pi}{\hbar} \; |\langle f|V|i\rangle|^2 \; \rho(E_f) \tag{17}$$

where V is the scattering potential and $\rho(E_f)$ is the density of final states. The integral $\langle f|V|i\rangle$ are the scattering matrix elements and will be denoted as $\overline{T}_{fi}$. The density of final states can be determined for three particles using a phase space argument.

If there are three final particles of mass m_i, momentum $\overline{k}_i$, and obey the constraint

$$\overline{k}_1 + \overline{k}_2 + \overline{k}_3 = 0 \tag{18}$$

then the system has 6 degrees of freedom. Assuming $\overline{k}_1$ and $\overline{k}_2$ are the independent momenta, the number of states in an interval of momenta $d\overline{k}_1 \; d\overline{k}_2$ is

$$dn = \frac{L^6 \; d\overline{k}_1 \; d\overline{k}_2}{(2\pi)^6} \tag{19}$$

where L^3 is a volume normalization constant, usually equal to $(2\pi)^3$. Planck's constant, $\hbar$ does not appear in Equation 19 because $\hbar = 1$ in atomic units. The density of states is defined as the number of states per energy, or

$$\rho(E_f) = \frac{dn}{dE_f} \tag{20}$$

where E_f is the total energy of the final state configuration, and is

given by

$$E_f = \frac{k_1^2}{2m_1} + \frac{k_2^2}{2m_2} + \frac{k_3^2}{2m_3} \qquad (21)$$

Conservation of energy requires

$$\int \delta \left(E_f - \sum_{i=1}^{3} \frac{k_i^2}{2m_i}\right) dE_f = 1 \qquad (22)$$

Multiplying Equation 22 by dn and integrating gives

$$\Delta n = \int_{\Delta n} dn = \frac{L^6}{(2\pi)^6} \int_{\Delta E_f} dE_f \int_{\Delta \bar{k}} d\bar{k}_1 \, d\bar{k}_2 \delta\left(E_f - \sum_{i=1}^{3} \frac{k_i^2}{2m_i}\right) \qquad (23)$$

This integral represents the total number of states in the energy range ΔE_f when all possible combinations of $d\bar{k}_2$ and $d\bar{k}_2$ are taken. In the limit as

$$\lim_{\Delta E_f \to 0} \frac{\Delta n}{\Delta E_f} = \frac{dn}{dE_f} \qquad (24)$$

implies that

$$\rho(E_f) = \frac{L^6}{(2\pi)^6} \int_{\Delta \bar{k}} d\bar{k}_1 \, d\bar{k}_2 \, \delta\left(E_f - \sum_{i=1}^{3} \frac{k_i^2}{2m_i}\right) \qquad (25)$$

which can be written as

$$\rho(E_f) = \left(\frac{L}{2\pi}\right)^6 \int k_1^2 \, dk_1 \, d\Omega_1 \, k_2^2 \, dk_2 \, d\Omega_2 \, \delta\left(E_f - \sum_{i=1}^{3} \frac{k_i^2}{2m_i}\right) \qquad (26)$$

It is now possible to integrate over dk_2 space using the properties of the delta function. The argument of the delta function can be rewritten using Equation 18, where

$$f(k_1, k_2) = E_f - \frac{k_1^2}{2\mu_{13}} - \frac{k_2^2}{2\mu_{23}} - \frac{2\bar{k}_1 \cdot \bar{k}_2}{2m_3} \qquad (27)$$

where μ_{ij} is the reduced mass of particles i and j. Using the identify

$$\delta(f(k_1, k_2)) = \sum_{\alpha=1} \frac{\delta(k_2 - k_2^\alpha)}{|f'(k_1, k_2)|\Big|_{k_2 = k_2^\alpha}} \qquad (28)$$

where there are n roots of $f(k_1, k_2)$ and k_2^α is a root, so that

$$f(k_1, k_2^\alpha) = 0 \qquad (29)$$

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The roots of $f(k_1, k_2^{\alpha})$ are found to be

$$k_2^{\pm} = \left[-\frac{k_1 \cos \psi}{m_3} \pm \sqrt{\frac{k_1^2 \cos^2 \psi}{m_3^2} + \frac{2E_f}{\mu_{23}} - \frac{k_1^2}{\mu_{23}\mu_{13}}} \right] \mu_{23} \qquad (30)$$

where ψ is the angle between $\bar{k}_1$ and $\bar{k}_2$. The negative root can be ignored because it is impossible for the magnitude of a real vector quantity to be negative. Therefore there is only one root for $f(k_1, k_2)$,

$$k_2^{+} = \left[-\frac{k_1 \cos \psi}{m_3} + \sqrt{\frac{k_1^2 \cos^2 \psi}{m_3^2} + \frac{2E_f}{\mu_{23}} - \frac{k_1^2}{\mu_{23}\mu_{13}}} \right] \mu_{23} \qquad (31)$$

The derivative of $f(k_1, k_2)$ is

$$f'(k_1, k_2) = \frac{df(k_1, k_2)}{dk_2} \qquad (32)$$

$$= -\frac{k_2}{\mu_{23}} - \frac{k_1 \cos \psi}{m_3} \qquad (33)$$

therefore

$$\left| f'(k_1, k_2) \right|_{k_2 = k_2^{+}} = \sqrt{\frac{k_1^2 \cos^2 \psi}{m_3^2} + \frac{2E_f}{\mu_{23}} - \frac{k_1^2}{\mu_{23}\mu_{13}}} \qquad (34)$$

Performing the integration of k_2, using Equation 28 gives the density of states to be

$$\rho(E_f) = \frac{k_1^2 \, dk_1 \, d\Omega_1 \, d\Omega_2 \, \mu_{23}^2 \left[-\frac{k_1 \cos \psi}{m_3} + \sqrt{\frac{k_1^2 \cos^2 \psi}{m_3} + \frac{2E_f}{\mu_{23}} - \frac{k_1^2}{\mu_{23}\mu_{13}}} \right]^2}{\sqrt{\frac{k_1^2 \cos^2 \psi}{m_3^2} + \frac{2E_f}{\mu_{23}} - \frac{k_1^2}{\mu_{23}\mu_{13}}}} \qquad (35)$$

The transition rate per unit solid angle due to a particle flux of intensity

$$I = \frac{V_i}{L^3} \qquad (36)$$

is

$$\frac{R}{d\Omega} = I \frac{d\sigma}{d\Omega} \qquad (37)$$

The differential cross section is then given by

$$\frac{d\sigma}{d\Omega_2} = \frac{2\pi L^3 |\overline{T}_{fi}|^2 \rho(E_f)}{V_i d\Omega_2} \tag{38}$$

where $\rho(E_f)$ is given in Equation 35.

For the specific problem to be evaluated the following substitutions are made

$$\overline{k}_1 = k_e$$

$$\overline{k}_2 = k_H$$

$$m_2 = m_3 = m_o$$

$$m_1 = m_e = 1$$

and E_f is given by Equation 15.

The Born Approximation

The scattering matrix elements, $\overline{T}_{fi}$, associated with the differential cross section depends upon the initial and final wave functions and also the scattering potential. If the scattering potential is different before and after the scattering, the potential can be written as a series, where

$$V = V_a + V_a G_o^+ V_b + V_a G_o^+ V_b G_o^+ V_a + --- \tag{39}$$

where V_a is the scattering potential before the collision, V_b is the scattering potential after the collision and

$$G_o^+ = \frac{1}{E_a + i\eta - H_o} \tag{40}$$

where G_o^+ is a form of a Green's function. This expansion of the potential gives rise to the Born series which is given by

$$\langle f|V|i\rangle = \langle f|V_a|i\rangle + \langle f|V_a G_o^+ V_b|i\rangle + ---- \tag{41}$$

where if all but the first term of the expansion are ignored, or

$$\langle f|V|i\rangle \simeq \langle f|V_a|i\rangle \tag{42}$$

is called the first Born Approximation. If the second term is included in the expansion it is then called the second Born Approximation, etc.

The first Born Approximation is valid as long as the incoming energy of the particle is much greater than the binding energy. In this study $W_o = 0.5$ hartrees, while $E_i \approx 10^4 - 10^6$ hartrees, therefore the first Born Approximation can be used.

At high energies the second term of the can be approximated as

$$T^{(2)} = \frac{1}{E_i} <f|V_a^2|i> \qquad (43)$$

An estimate of the correction supplied by the second term is found by looking at the ratio of $T^{(2)}$ to $T^{(1)}$, or

$$\left| \frac{T^{(2)}}{T^{(1)}} \right| = \frac{1}{E_i} \left| \frac{<f|V_a^2|i>}{<f|V_a|i>} \right| \qquad (44)$$

and for $E_i \sim 10^5 - 10^6$,

$$\left| \frac{T^{(2)}}{T^{(1)}} \right| = \frac{1}{10^6} \left| \frac{<f|V_a^2|i>}{<f|V_a|i>} \right| \qquad (45)$$

and in all probability

$$\left| \frac{<f|V_a^2|i>|}{<f|V_a|i>|} \right| \sim 10 \qquad (46)$$

Then

$$|T^{(2)}| \sim 10^{-4}|T^{(1)}| \qquad (47)$$

and the first term of the Born Series can be used to calculate the differential cross section, accurately.

III. The Hamiltonian, Scattering Potential, and Particle Wave Functions

The motion and subsequent wave functions for a system of particles can be found by solving the quantum mechanical Hamiltonian of the system. This chapter develops the Hamiltonian of the total system and from it the scattering potential, and initial and final wave functions are obtained. This chapter concludes with a discussion of the antisymmeterization of the final wave function.

The Total Hamiltonian

The motion of the particles in the center of mass frame is described completely by the total Hamiltonian of the system. In the case of a H^- ion colliding with a H atom, the Hamiltonian is given by

$$H = \frac{P_1^2}{2M_p} + \frac{P_2^2}{2M_p} + \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + \frac{p_3^2}{2m} -$$

$$\frac{1}{|\overline{R}_1 - \overline{X}_1|} - \frac{1}{|\overline{R}_2 - \overline{X}_2|} - \frac{1}{|\overline{R}_2 - \overline{X}_3|} + \frac{1}{|\overline{X}_2 - \overline{X}_3|} +$$

$$\frac{1}{|\overline{R}_1 - \overline{R}_2|} + \frac{1}{|\overline{X}_1 - \overline{X}_2|} + \frac{1}{|\overline{X}_1 - \overline{X}_3|} - \frac{1}{|\overline{R}_1 - \overline{X}_2|} -$$

$$\frac{1}{|\overline{R}_1 - \overline{X}_3|} - \frac{1}{|\overline{R}_2 - \overline{X}_1|} \tag{48}$$

where the first two terms represent the kinetic energy of the two protons, the next three terms represent the kinetic energy of the electrons and the last ten terms represents the electrostatic potential between the particles. The position vectors in the electrostatic potential terms are depicted in Figure 1, where $\overline{R}_i$ is the position vector of the
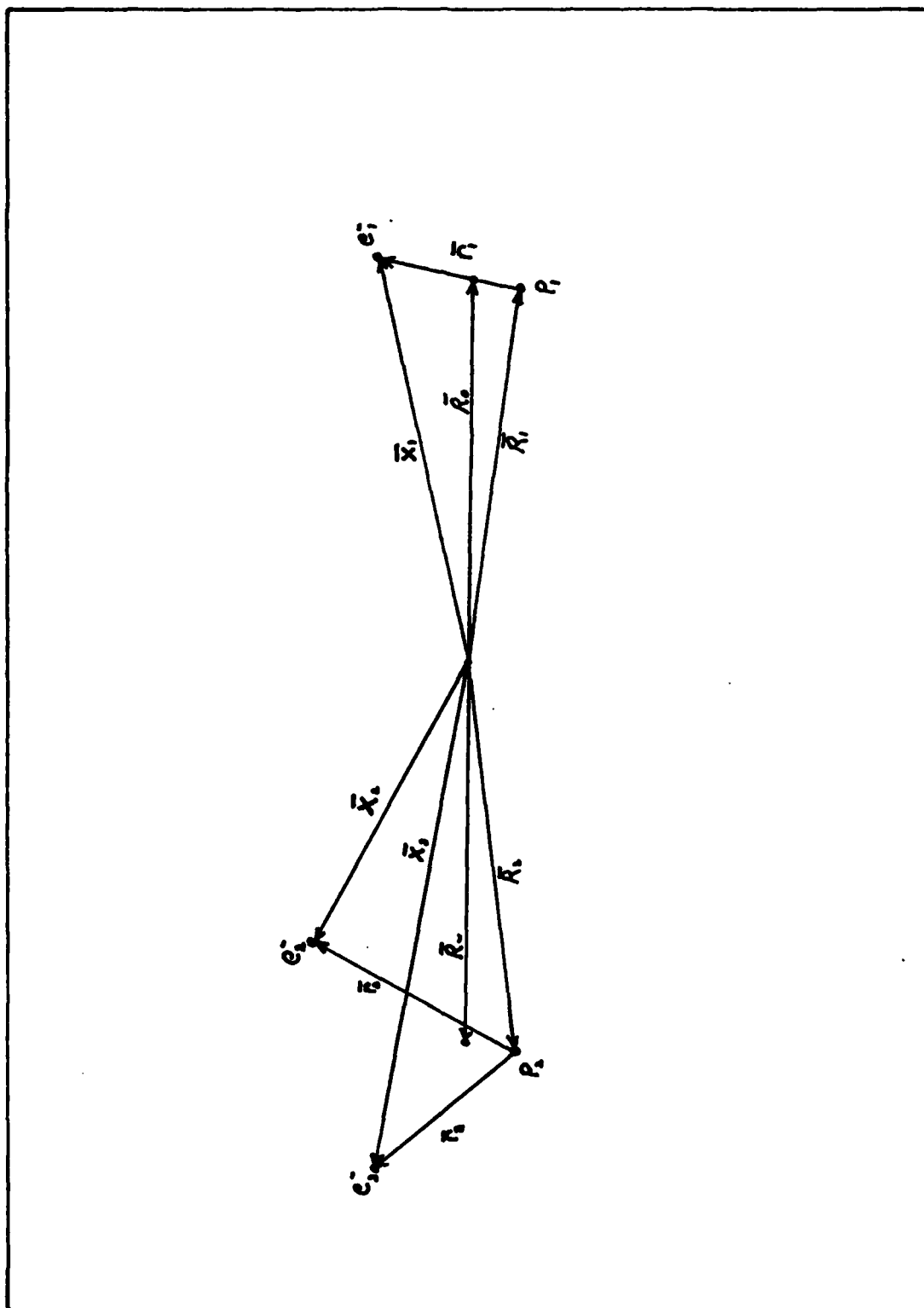
Figure 1. Position Vector for H-H⁻ Confoguration

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i^{th} proton and $\overline{X}_i$ is the position vector of the jth electron. The total Hamiltonian can now be used to find the particle Hamiltonians and the scattering potential before and after the collision.

When the particles are separated and do not interact, the initial configuration consists of a H⁻ ion and a H atom. The Hamiltonian for the H atom is given simply by

$$K_H = \frac{P_1^{\,2}}{2M_p} + \frac{P_1^{\,2}}{2m} - \frac{1}{|\overline{R}_1 - \overline{X}_1|} \tag{49}$$

assuming electron 1 and proton 1 are in the H target atom initially. The H⁻ ion's Hamiltonian is the three-body Hamiltonian

$$K_{H^-} = \frac{P_2^{\,2}}{2M_p} + \frac{P_2^{\,2}}{2m_e} + \frac{P_3^{\,2}}{2m_e} + \frac{1}{|\overline{X}_3 - \overline{X}_3|} - \frac{1}{|\overline{R}_2 - \overline{X}_2|} - \frac{1}{|\overline{R}_2 - \overline{X}_3|} \tag{50}$$

assuming proton 2 and electron 2 and 3 are in the H⁻ ion. In reality the designation of each particle *is for accounting purposes only*, and comes into play when there is an exchange of particles.

The scattering potential, V_a, can be found by subtracting the particle Hamiltonians from the total Hamiltonian or

$$V_a = H - K_H - K_{H^-} \tag{51}$$

$$= \frac{1}{|\overline{R}_1 - \overline{R}_2|} + \frac{1}{|\overline{X}_1 - \overline{X}_2|} + \frac{1}{|\overline{X}_1 - \overline{X}_3|} -$$

$$\frac{1}{|\overline{R}_1 - \overline{X}_2|} - \frac{1}{|\overline{R}_1 - \overline{X}_3|} - \frac{1}{|\overline{X}_1 - \overline{R}_1|} \tag{52}$$

To simplify notation, the following convention will be used

$$V_{ij} = \frac{1}{|\overline{X}_i - \overline{X}_j|} \tag{53}$$

$$V_j^{\;i} = \frac{1}{|\overline{R}_i - \overline{X}_j|} \qquad (54)$$

$$V_p = \frac{1}{|\overline{R}_1 - \overline{R}_2|} \qquad (55)$$

The scattering potential is now written as

$$V_a = V_p + V_{12} + V_{13} - V_2^{\;1} - V_3^{\;1} - V_1^{\;2} \qquad (56)$$

After the collision, when the particles are separated and do not interact, there are two H atoms and one free electron. The Hamiltonian for the H target atom is

$$K_H^{'} = \frac{P_\alpha^{\;2}}{2M_p} + \frac{P_i^{\;2}}{2m_e} - V_i^{\;\alpha} \qquad (57)$$

where α represents the αth proton and i represents the ith electron. The Hamiltonian for the resultant H atom is

$$K_R = \frac{P_\beta^{\;2}}{2M_p} + \frac{P_j^{\;2}}{2m_e} - V_j^{\;\beta} \qquad (58)$$

where proton β and electron j are in the resultant H atom. The Hamiltonian for the free electron k is

$$K_e^{'} = \frac{P_k^{\;2}}{2m_e} \qquad (59)$$

The above notation was used to account for exchange of the particles during the collision. In the above cases if $\alpha = 1$, $\beta = 2$ or if $\beta = 1$, $\alpha = 2$, and i, j, and k are the permutations of 1, 2 and 3. All permutations of the indices are presented in Table 1. The permutation of the particles is discussed in further detail when the final wave function is formulated.

Once again the scattering potential is found using

$$V_b = H - K_H^{'} - K_R^{'} - K_e^{'} \qquad (60)$$

$$= V_p + V_{ij} + V_{ik} + V_{jk} - V_j^{\;\alpha} - V_k^{\;\alpha} - V_i^{\;\beta} - V_k^{\;\beta} \qquad (61)$$

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Table 1				
Permutations of Particles in Final State				
H (Target)		H (Resultant)		e⁻ (Free)
e^-	P	e^-	P	e^-
1	1	2	2	3
1	1	3	2	2
2	1	1	2	3
2	1	3	2	1
3	1	1	2	2
3	1	2	2	1
1	2	2	1	3
1	2	3	1	2
2	2	1	1	3
2	2	3	1	1
3	2	1	1	2
3	2	2	1	1

Therefore $V_a \neq V_b$, that is the scattering potentials are different before and after the collision. It can be shown that the scattering matrix, $\overline{T}_{fi}$, is the same whether V_a or V_b is used. $\overline{T}_{fi}$, is given by

$$\overline{T}_{fi} = \langle f | V_a | i \rangle \tag{62}$$

Using Equation 51 this can be written as

$$\overline{T}_{fi} = \langle f | (H - K_H - K_{H^-}) i \rangle \tag{63}$$

and

$$(K_H + K_{H^-}) | i \rangle = E_a | i \rangle \tag{64}$$

therefore Equation 63 becomes

$$\overline{T}_{fi} = \langle f | (H - E_a) \, i \rangle \tag{65}$$

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Since H and E_a are both hermitian operators this can be written as

$$\overline{T}_{fi} = \langle(H - E_a)f|i\rangle \qquad (66)$$

But on the energy shell $E_a = E_b$ (Conservation of Energy),

$$\overline{T}_{fi} = \langle(H - E_b)f|i\rangle \qquad (67)$$

and using Equation 60 this is

$$\overline{T}_{fi} = \langle(H - K_H' - K_R' - K_e')f|i\rangle \qquad (68)$$

or

$$\overline{T}_{fi} = \langle V_b f|i\rangle \qquad (69)$$

Since V_b is also hermitian, Equation 69 is

$$\overline{T}_{fi} = \langle f|V_b|i\rangle \qquad (70)$$

Therefore

$$\overline{T}_{fi} = \langle f|V_a|i\rangle = \langle f|V_b|i\rangle \qquad (71)$$

and the scattering potential will be

$$V = V_a = V_b + V_{12} + V_{13} - V_2{}^1 - V_3{}^1 - V_1{}^2 \qquad (72)$$

Initial Wavefunction

The initial particles wavefunctions are obtained by obtaining solutions to the particle Hamiltonians. The initial wavefunction is the product of the initial particle wavefunctions. The initial wave function of the H target atom is

$$\psi_H(1s,1) = N_H \exp(-r_1)\exp(-i\overline{k}_-\cdot\overline{R}_o)U_{\nu_1}(s_1)U_{\mu_1}(P_1) \qquad (73)$$

where N_H is a normalization constant equal to $(8\pi^2)^{-\frac{1}{2}}$, the first term represents the atomic wavefunction for an electron in the ground state

of a H atom, the second term represents the plane wave associated with the center of mass of the H atom, the third and fourth terms represent the spin functions for the electron and proton, respectively. Equation 73 written in parabolic coordinates is

$$\psi_H(1s;1) = N_H \exp(-\tfrac{1}{2}(\xi + \eta))\exp(-i\overline{k}\cdot\overline{R}_0)U_{\nu_1}(s_1)U_{\mu_1}(P_1) \qquad (74)$$

The wave function for the H^- ion is a numerical solution to the three body Hamiltonian (Equation 50). There are many numerical solutions in the literature. For this study, a simple two parameter wavefunction will be used (Ref 6:625) in order that the spatial integration to be done analytically. The H^- ion is given by

$$\psi_{H^-}(1s^2;2,3) = N_{H^-} \left[\exp(-\alpha r_2 - \beta r_3) + \exp(-\alpha r_3 - \beta r_2)\right] \cdot$$
$$\exp(i\overline{k}_-\cdot\overline{R}_-)\left[U_{\frac{1}{2}}(s_3)U_{-\frac{1}{2}}(s_3) - U_{\frac{1}{2}}(s_2)U_{-\frac{1}{2}}(s_2)\right] \cdot$$
$$U_{\mu_2}(P_2) \qquad (75)$$

where N_{H^-} is a normalization constant equal to $\sqrt{\dfrac{\alpha^3\beta^3}{32\pi^5}}$, the first term in brackets is the orbital wave function for the H^- electrons with $\alpha = 1.03923$ and $\beta = 0.283221$, the second term represents the plane wave associated with the center of mass of the H^- ion, the third term represents the antisymmetric spin functions of the two electrons while the fourth term represents the protons spin function. The total initial wave function is then

$$|i> = \psi_H(1s:1)\,\psi_H(1s^2:2,3) \qquad (76)$$

Final Wavefunction

After the collision the three particles have wavefunctions that correspond to the solution of the corresponding particle Hamiltonian.

The H target atom in the Nth excited state has a wave function, in parabolic coordinates, given by

$$\psi_H(N;i,\alpha) = \frac{N_H'}{N^2} \exp(-\frac{1}{2}(\xi + n)/N)F(-n_1,1,\xi/N) \cdot$$

$$F(-n_2,1,\eta/N)\exp(-i(\overline{k}_H + \overline{k}_e)\cdot\overline{R}_o')U_{\nu_i}'(s_i)$$

$$U_{\mu_i}'(P_2) \tag{77}$$

where $N_H' = (8\pi^2)^{-\frac{1}{2}}$, $F(-n_1,1,\xi/N)$, and $F(-n_2,1,\eta/N)$ are confluent hypergeometric functions and $N = n_1 + n_2 + 1$. The resultant H atom has a wave function of the form

$$\psi_R(1s;j,\beta) = N_R' \exp(-r_j)\exp(i\overline{k}_H\cdot\overline{R}_H)U_{\nu_2}'(s_j)U_{\mu_2}'(P_\beta) \tag{78}$$

where $N_R' = (8\pi^2)^{-\frac{1}{2}}$, if the final state is nl = 1s, or

$$\psi_R(1s;j,\beta) = N_R'(2 - r_j)\exp(-r_j/2)\exp(i\overline{k}_H\cdot\overline{R}_H) \cdot$$

$$U_{\nu_2}'(s_j)U_{\mu_2}'(P_\beta) \tag{79}$$

where $N_R' = (256\pi^2)^{-\frac{1}{2}}$ if the final state is nl = 2s. The wave function for the free electron k is simply

$$\psi_e(k) = (2\pi)^{-3/2} \exp(i\overline{k}_e\cdot\overline{r}_e)\cdot U_{r_3}'(s_k) \tag{80}$$

Because the particles could have exchanged positions it is necessary to antisymmeterize the final wave function. Therefore the total final wave function is

$$\psi_f = \frac{1}{\sqrt{12}} \begin{vmatrix} (r_1,\nu_1' ;P_1,\mu_1') & (r_1, \nu_1';P_2,\mu_2')' & \{r_1,\nu_1'\} \\ (r_2,\nu_2' ;P_1,\mu_1') & (r_2, \nu_2'; P_2,\mu_2')' & \{r_2,\nu_2'\} \\ (r_3,\nu_3' ;P_1,\mu_1') & (r_3, \nu_3'; P_2,\mu_2')' & \{r_3,\nu_3'\} \end{vmatrix}$$

$$\frac{1}{\sqrt{12}} \begin{vmatrix} (r_1,\nu_1' ;P_2,\mu_2') & (r_1,\nu_1' ;P_1,\mu_1')' & \{r_1,\nu_1'\} \\ (r_2,\nu_2' ;P_2,\mu_2') & (r_2,\nu_2' ;P_1,\mu_1')' & \{r_2,\nu_2'\} \\ (r_3,\nu_3' ;P_2,\mu_2') & (r_3,\nu_3' ;P_1,\mu_1')'' & \{r_3,\nu_3'\} \end{vmatrix} \tag{81}$$

where $(r_i,\nu_i';P_\alpha,\mu_\alpha')$ is the wavefunction of the H target atom with electron i and proton α, $(r_j, \nu_j'; P_\beta, \mu_\beta')'$ is the wavefunction of the resultant H atom with electron j and proton β, and $\{r_k,\nu_k'\}$ is the wavefunction for the free electron k. Using the scattering potential, V_a, the initial wave function and the final wavefunction the Scattering Matrix $\overline{T}_{fi}$ can now be obtained.

IV.   The Scattering Matrix, T_{fi}

This chapter develops and evaluates the scattering matrix, $\overline{T}_{fi}$, for use in the differential cross section. The total scattering matrix is derived and each term discussed in terms of particles exchanged. The spin states of the initial and final configuration are averaged and summed over, respectively, to obtain the scattering matrix, T_{fi}. Finally, the terms in the scattering matrix, T_{fi}, are evaluated and discussed.

Scattering Matrix, $\overline{T}_{fi}$

The total scattering matrix, $\overline{T}_{fi}$, is developed using the first term in the Born Series and the initial and final wavefunctions and scattering potential developed in the previous chapter. The scattering matrix is given by

$$\overline{T}_{fi} = <f|V|i> \tag{82}$$

and using the identity,

$$<U_{\nu_i}(s_i)\ U_{\nu_i}(s_i)> = \delta_{\nu_i \nu_i'} \tag{83}$$

where $\delta_{\nu_i,\nu_i'}$ is the Kronecker delta, the scattering matrix is given by

$$
\begin{aligned}
T_{fi} = \{ &[\delta_{\nu_1,\nu_1'}\ \delta_{\frac{1}{2},\nu_2'}\ \delta_{-\frac{1}{2},\nu_3} - \delta_{\nu_1,\nu_1'}\ \delta_{-\frac{1}{2},\nu_2'}\ \delta_{\frac{1}{2},\nu_3'}](1,2,3|V|1,2,3) + \\
&[\delta_{\nu_1,\nu_2'}\ \delta_{\frac{1}{2},\nu_3'}\ \delta_{-\frac{1}{2},\nu_1'} - \delta_{\nu_1,\nu_2'}\ \delta_{-\frac{1}{2},\nu_3'}\ \delta_{\frac{1}{2},\nu_1'}](3,1,2|V|1,2,3) + \\
&[\delta_{\nu_1,\nu_3'}\ \delta_{\frac{1}{2},\nu_1'}\ \delta_{-\frac{1}{2},\nu_2'} - \delta_{\nu_1,\nu_3'}\ \delta_{-\frac{1}{2},\nu_1'}\ \delta_{\frac{1}{2},\nu_2'}](2,3,1|V|1,2,3) + \\
&[\delta_{\nu_1,\nu_1'}\ \delta_{\frac{1}{2},\nu_2'}\ \delta_{-\frac{1}{2},\nu_3'} - \delta_{\nu_1,\nu_1'}\ \delta_{-\frac{1}{2},\nu_2'}\ \delta_{\frac{1}{2},\nu_3'}](1,3,2|V|1,2,3) + \\
&[\delta_{\nu_1,\nu_2'}\ \delta_{\frac{1}{2}\cdot\nu_3'}\ \delta_{-\frac{1}{2},\nu_1'} - \delta_{\nu_1,\nu_2'}\ \delta_{-\frac{1}{2},\nu_3'}\ \delta_{\frac{1}{2},\nu_1'}](2,1,3|V|1,2,3) +
\end{aligned}
$$

$$[\delta_{\nu_1,\nu_3'}\,\delta_{\frac{1}{2},\nu_1'}\quad \delta_{-\frac{1}{2},\nu_2'} - \delta_{\nu_1,\nu_3'}\,\delta_{-\frac{1}{2},\nu_1'}\,\delta_{\frac{1}{2},\nu_2'}](3,2,1|V|1,2,3)\} \ .$$

$$\{\delta_{\mu_1,\mu_1'}\,\delta_{\mu_2,\mu_2'} - \delta_{\mu_1,\mu_2'}\,\delta_{\mu_2,\mu_1'}\} \tag{84}$$

where $(i,j,k\ V\ 1,2,3)$ represents the spatial integration of

$$(i,j,k|V|1,2,3) = \int \psi_H(N,i,\alpha)\psi_R(nl,j,\beta)\psi_e(k)\cdot V\cdot$$

$$\psi_H(1s,1)\psi_{H^-}(1s^2,2,3)\ d\bar{\tau} \tag{85}$$

The terms in the scattering matrix can be defined in terms of exchanged particles. This leaves six basic scattering matrices. In the case of no exchange, or the direct scattering matrix, $\bar{T}$, the scattering matrix is given by

$$\bar{T}_d = [\delta_{\nu_1,\nu_1'}\,\delta_{\frac{1}{2},\nu_2'}\quad \delta_{-\frac{1}{2},\nu_3'} - \delta_{\nu_1,\nu_1'}\,\delta_{-\frac{1}{2},\nu_2'}\,\delta_{\frac{1}{2},\nu_3'}]\cdot(\delta_{\mu_1,\mu_1'}\,\delta_{\mu_2,\mu_2'})\cdot$$

$$(1,2,3 + 1,3,2|V|1,2,3) \tag{86}$$

The scattering matrix that accounts for exchange of electrons between the final H target and H resultant atoms is

$$\bar{T}_{e,H} = [\delta_{\nu_1,\nu_2'}\,\delta_{\frac{1}{2},\nu_3'}\,\delta_{-\frac{1}{2},\nu_1'} - \delta_{\nu_1,\nu_2'}\,\delta_{-\frac{1}{2},\nu_3'}\,\delta_{\frac{1}{2},\nu_1'}]\cdot(\delta_{\mu_1,\mu_1'}\,\delta_{\mu_2,\mu_3'})\cdot$$

$$(3,1,2 + 2,1,3|V|1,2,3) \tag{87}$$

The scattering matrix that accounts for exchange of electrons between the H target atom and the free electron is

$$\bar{T}_{e,f} = [\delta_{\nu_1,\nu_3'}\,\delta_{\frac{1}{2},\nu_1'}\,\delta_{-\frac{1}{2},\nu_2'} - \delta_{\nu_1,\nu_3'}\,\delta_{-\frac{1}{2},\nu_1'}\,\delta_{\frac{1}{2},\nu_2'}]\cdot(\delta_{\mu_1,\mu_1'}\,\delta_{\mu_2,\mu_2})\cdot$$

$$(2,3,1 + 3,2,1|V|1,2,3) \tag{88}$$

The scattering matrix that accounts for exchange of hydrogen atoms between the final H target atom and H resultant atom is

$$\bar{T}_H = [\delta_{\nu_1,\nu_2'}\,\delta_{\frac{1}{2},\nu_3'}\,\delta_{-\frac{1}{2},\nu_1'} - \delta_{\nu_1,\nu_2'}\,\delta_{-\frac{1}{2},\nu_3'}\,\delta_{\frac{1}{2},\nu_1'}]\cdot(\delta_{\mu_1,\mu_2'}\,\delta_{\mu_2,\mu_1'})\cdot$$

$$(3,1,2 + 2,1,3|V|1,2,3) \tag{89}$$

The scattering matrix that accounts for exchange of protons in the

hydrogen atoms and electrons between the target atom and free electron is

$$\overline{T}_{p,f} = [\delta_{\nu_1,\nu_3'} \delta_{\frac{1}{2},\nu_1'} \delta_{-\frac{1}{2},\nu_2'} - \delta_{\nu_1,\nu_3'} \delta_{-\frac{1}{2},\nu_1'} \delta_{+\frac{1}{2},\nu_2'}] \cdot (\delta_{\mu_1,\mu_2'} \delta_{\mu_2,\mu_1'}) \cdot$$
$$(2,3,1 + 3,2,1|V|1,2,3) \tag{90}$$

The scattering matrix that accounts for exchange of protons between the

final H atom is

$$\overline{T}_{p} = [\delta_{\nu_1,\nu_1'} \delta_{\frac{1}{2},\nu_2'} \delta_{-\frac{1}{2},\nu_3'} - \delta_{\nu_1,\nu_2'} \delta_{-\frac{1}{2},\nu_2'} \delta_{\frac{1}{2},\nu_3'}] \cdot (\delta_{\mu_1,\mu_2'} \delta_{\mu_2,\mu_1'}) \cdot$$
$$(1,2,3 + 1,3,2|V|1,2,3) \tag{91}$$

In all cases the last term represents the spatial integration of the

wave function as shown in Equation 84. The total scattering matrix

is now written as

$$\overline{T}_{fi} = \overline{T}_d + \overline{T}_{e,H} + \overline{T}_{ef} - \overline{T}_p - \overline{T}_H - \overline{T}_{p,f} \tag{92}$$

Averaging and Summing Over Spin States

The scattering matrix, $\overline{T}_{fi}$, depends explicitly on the spin of the

particles before and after the collision. To remove this dependence

it is necessary to sum over the final spin states and average over the

initial spin states. Table 2 represents the possible spin configura-

tions and the associated scattering matrix for each spin configuration.

In Table 2, T_A represents the spatial integration of the scattering

matrix T_A, such as

$$T_d = (3,1,2 + 2,1,3|V|1,2,3) \tag{93}$$

Not all spin states have been included, but it can easily be shown that

all other spin states are just representations of those in Table 2.

The scattering matrix for the differential cross section is then

<div align="center">

Table 2

Spin Configurations and Associated Scattering Matrices

</div>

INITIAL					FINAL					$\lvert T \rvert$
e^-			p		e^-			p'		
ν_1	ν_2	ν_3	μ_1	μ_2	ν_1'	ν_2'	ν_3'	μ_1'	μ_2'	
+	+	−	+	+	+	+	−	+	+	$\lvert T_d - T_{e,H} - T_p + T_H \rvert$
+	+	−	+	+	+	−	+	+	+	$\lvert T_d - T_{e,f} - T_p + T_{p,f} \rvert$
+	+	−	+	+	−	+	+	+	+	$\lvert T_{e,H} - T_{e,f} + T_{p,f} - T_H \rvert$
+	+	−	+	−	+	+	−	+	−	$\lvert T_d - T_{e,H} \rvert$
+	+	−	+	−	+	−	+	+	−	$\lvert T_d - T_{e,f} \rvert$
+	+	−	+	−	−	+	+	+	−	$\lvert T_{e,H} - T_{e,f} \rvert$
+	+	−	+	−	+	+	−	−	+	$\lvert T_p - T_H \rvert$
+	+	−	+	−	+	−	+	−	+	$\lvert T_p - T_{p,f} \rvert$
+	+	−	+	−	−	+	+	−	+	$\lvert T_H - T_{p,f} \rvert$

$$\lvert T_{fi} \rvert = \frac{1}{2} \{ \lvert T_d - T_{e,H} - T_p + T_H \rvert + \lvert T_d - T_{e,f} - T_p + T_{p,f} \rvert +$$

$$\lvert T_{e,H} - T_{e,f} + T_{p,f} - T_H \rvert + \lvert T_d - T_{e,H} \rvert + \lvert T_d - T_{p,f} \rvert +$$

$$\lvert T_{e,H} - T_{e,f} \rvert + \lvert T_p - T_H \rvert + \lvert T_p - T_{p,f} \rvert + \lvert T_H - T_{p,f} \rvert \} \quad (94)$$

The evaluation of each of the scattering matrices is presented in the next 6 sections.

Evaluation of Direct Scattering Matrix, T_d

The scattering matrix associated with no exchange of particles is the direct scattering matrix and is given by the spatial terms of

$$T_d = \sqrt{\frac{1}{12}} \int \psi_H^*(N;1.1)\{\psi_R^*(nl,2,2)\psi_e^*(3) + \psi_R^*(nl,3,2)\psi_e^*(2)\} \cdot$$

$$V \cdot \psi_H(1s;1)\psi_H-(1s^2 12,3)d\tau \quad (95)$$

where $\psi_H^*(N;1,1)$, $\psi_R^*(nl;j,\beta)$, $\psi_e^*(k)$, $\psi_H(1s;1)$, $\psi_H(1s^2;2,3)$ and V are described by Equations 77, 78, 80, 74, 75, and 72, respectively. Written explicitly this is

$$T_d = \frac{1}{\sqrt{12}} \int \frac{N_H'}{N^2} \exp\left(-\frac{1}{2n}(\xi+\eta)\right) F(-n_1,1,\xi/N) F(-n_2,1,\eta/N) \cdot$$

$$\{(2\pi)^{-\frac{1}{2}} N_R' \chi^*(nl,2) \exp(-i\overline{k}_H \cdot \overline{R}_H) \exp(-i\overline{k}_e \cdot \overline{r}_e) +$$

$$\{(2)^{-\frac{1}{2}} N_R' \chi^*(nl,3) \exp(-i\overline{k}_H \cdot \overline{R}_H) \exp(-i\overline{k}_e \cdot \overline{r}_e)\} \cdot$$

$$\{V_p + V_{12} + V_{13} - V_2^{\ 1} - V_3^{\ 1} - V_1^{\ 2}\} \cdot$$

$$N_H \exp(-r_1) \exp(-i\overline{k}_- \cdot \overline{R}_o + i(k_H + \overline{k}_e) \cdot \overline{R}_o') \cdot$$

$$N_{H^-} \exp(-\alpha r_2 - \beta r_3) + \exp(-\alpha r_3 - \beta r_2) \ \exp(i\overline{k}_- \cdot \overline{R}_-) d\overline{\tau} \qquad (96)$$

where all terms are defined in Chapter 4, and $\chi^*(nl,i)$ is the hydrogen wave function for the nl state. Denoting

$$\psi_H^*(N,1) = \frac{N_H'}{N^2} \exp\left(-\frac{1}{2n}(\xi+\eta)\right) F(-n_1,1,\xi/N) F(-n_2,1,\eta/N) \qquad (97)$$

$$\psi_H(1s,1) = N_H \exp(-r_1) \qquad (98)$$

$$\chi_{H^-}(1s^2;2,3) = N_{H^-} \exp(-\alpha r_2 - \beta r_3) + \exp(-\alpha r_3 - \beta r_2) \qquad (99)$$

Equation 96 can be written as

$$T_d = \frac{(2\pi)^{-15/2}}{\sqrt{12}} \int \psi_H^*(N;1) \cdot \psi_H(1s,1) \chi_{H^-}(1s^2;2,3) \cdot$$

$$\{\chi^*(nl,2) \exp(-i'(\overline{k}_H \cdot \overline{R}_H + \overline{k}_e \cdot \overline{r}_e)) +$$

$$\chi^*(nl,3) \exp(-i(\overline{k}_H \cdot \overline{R}_H + \overline{k}_e \cdot \overline{r}_e))\} \cdot$$

$$\exp(i\overline{k}_- \cdot (\overline{R}_- - \overline{R}_o) + i(\overline{k}_e + \overline{k}_H) \cdot \overline{R}_o') \cdot$$

$$V_p + V_{12} + V_{13} - V_2^{\ 1} - V_3^{\ 1} - V_1^{\ 2} \ d\overline{\tau} \qquad (100)$$

The factor of $(2\pi)^{-15/2}$ is from the constants in Equations 97, 98, and 99 to account for normalization of the plane waves in the integral. Then $N_H' = \pi^{-\frac{1}{2}}$, $N_H = \pi^{-\frac{1}{2}}$, $N_{H^-} = \sqrt{\frac{\alpha^3 \beta^3}{2^2 \pi^2}}$ and $N_R' = \pi^{-\frac{1}{2}}$ if nl = 1s or

$N_R^{'} = (32\pi)^{-\frac{1}{2}}$ if nl = 2s. Making a change of coordinates described in Appendix A, Equation 99 can be written as

$$T_d = \frac{(2\pi)^{-15/2}}{\sqrt{12}} \int \psi_H^*(N;1)\psi_H(1s;1)\chi_H^-(1s^2;2,3) \cdot$$

$$\{\chi^*(nl,3)\exp(-i\overline{k}_H \cdot (-\tfrac{1}{3}\overline{r}_2 + \tfrac{2\epsilon-1}{3(1+\epsilon)}\overline{r}_3)) \cdot$$

$$\exp(-i\overline{k}_e \cdot (\tfrac{2}{3}\overline{r}_2 - \tfrac{1}{3}\overline{r}_3)) + \chi^*(nl,2) \cdot$$

$$\exp(-i\overline{k}_H \cdot (-\tfrac{1}{3}\overline{r}_3 + \tfrac{2\epsilon-1}{3(1+\epsilon)}\overline{r}_2))\exp(-i\overline{k}_e - (\tfrac{2}{3}\overline{r}_3 - \tfrac{1}{3}\overline{r}_2))\} \cdot$$

$$\exp(i\overline{k}_- \cdot (\tfrac{\epsilon-1}{3(1+2\epsilon)}(\overline{r}_2 + \overline{r}_3) - \tfrac{\epsilon-1}{2(1+\epsilon)}\overline{r}_1)) \cdot$$

$$\exp(i(\overline{k}_H + \overline{k}_e) \cdot (\tfrac{\epsilon-1}{2(1+\epsilon)}\overline{r}_1) \cdot \exp(i\overline{K} \cdot (\overline{\tau}_2 - \overline{\tau}_1)) \cdot$$

$$\left[|\overline{\tau}_1 - \overline{\tau}_2 - \tfrac{1}{2}\overline{r}_1 + \tfrac{1}{3}\overline{r}_2 + \tfrac{1}{3}\overline{r}_3|^{-1} + |\overline{\tau}_1 - \overline{\tau}_2 + \tfrac{1}{2}\overline{r}_1 - \right.$$

$$\tfrac{2}{3}\overline{r}_2 + \tfrac{1}{3}\overline{r}_3|^{-1} +$$

$$|\overline{\tau}_1 - \overline{\tau}_2 + \tfrac{1}{2}\overline{r}_1 + \tfrac{1}{3}\overline{r}_2 - \tfrac{2}{3}\overline{r}_3|^{-1} - |\overline{\tau}_1 - \overline{\tau}_2 - \tfrac{1}{2}\overline{r}_1 -$$

$$\tfrac{2}{3}\overline{r}_2 + \tfrac{1}{3}\overline{r}_3|^{-1} -$$

$$|\overline{\tau}_1 - \overline{\tau}_2 - \tfrac{1}{2}\overline{r}_1 + \tfrac{1}{3}\overline{r}_2 - \tfrac{2}{3}\overline{r}_3|^{-1} - |\overline{\tau}_1 - \overline{\tau}_2 + \tfrac{1}{2}\overline{r}_1 -$$

$$\left. \tfrac{1}{3}\overline{r}_2 + \tfrac{1}{3}\overline{r}_3|^{-1} \right] \cdot$$

$$d\overline{\tau}_1 \, d\overline{\tau}_2 \, d\overline{r}_1 \, d\overline{r}_2 \, d\overline{r}_3 \tag{101}$$

where $\overline{K} = \overline{k}_- - \overline{k}_H - \overline{k}_e$. To simplify the notation, the following convention is used,

$$\psi_H^{'*}(N;1) = \psi_H^*(N;1)\exp(+i(\overline{k}_H + \overline{k}_e) \cdot \tfrac{\epsilon-1}{2(1+\epsilon)}\overline{r}_1) \tag{102}$$

$$\chi^{'*}(nl;i,j) = \chi^*(nl;i)\exp(i\,\overline{r}_i \cdot (\tfrac{1}{3}\overline{k}_3 - \tfrac{2\epsilon-1}{3(1+\epsilon)}\overline{k}_H) \cdot$$
$$\exp(i\,\overline{r}_j \cdot (\tfrac{1}{3}k_H - \tfrac{2}{3}\overline{k}_e)) \tag{103}$$

$$\psi_H^{'}(1s;1) = \psi_H(1s;1)\exp(-i\,\overline{k}_- \cdot \tfrac{\epsilon-1}{2(1+\epsilon)}\overline{r}_1) \tag{104}$$

and

$$\psi_H'(1s^2;2,3) = \chi_{H^-}(1s^2;2,3)\exp(i\overline{k}_- \cdot \frac{\epsilon-1}{3(1+2\epsilon)} (\overline{r}_2 + \overline{r}_3)) \qquad (105)$$

Using this notation Equation 101 is written as

$$T_d = \frac{(2\pi)^{-15/2}}{\sqrt{12}} \int \psi_H'^*(N;1)\psi_H'(1s;1)\chi_{H^-}'(1s^2;2,3) \cdot$$

$$\{\chi'^*(nl;3,2) + \chi'^*(nl;2,3)\}\cdot$$

$$\left[\mid \overline{\tau}_1 - \overline{\tau}_2 - \frac{1}{2}\overline{r}_1 + \frac{1}{3}\overline{r}_2 + \frac{1}{3}r_3 \mid^{-1} + \mid \overline{\tau}_1 - \overline{\tau}_2 + \frac{1}{2}\overline{r}_1 - \frac{2}{3}\overline{r}_2 \right.$$

$$\left. + \frac{1}{3}\overline{r}_3 \mid^{-1} + \right.$$

$$\mid \overline{\tau}_1 - \overline{\tau}_2 + \frac{1}{2}\overline{r}_1 + \frac{1}{3}\overline{r}_2 - \frac{2}{3}\overline{r}_3 \mid^{-1} - \mid \overline{\tau}_1 - \overline{\tau}_2 - \frac{1}{2}\overline{r}_1 -$$

$$\frac{2}{3}\overline{r}_2 + \frac{1}{3}\overline{r}_3 \mid^{-1} -$$

$$\mid \overline{\tau}_1 - \overline{\tau}_2 - \frac{1}{2}\overline{r}_1 + \frac{1}{3}\overline{r}_2 - \frac{2}{3}\overline{r}_3 \mid^{-1} - \mid \overline{\tau}_1 - \overline{\tau}_2 + \frac{1}{2}\overline{r}_1 -$$

$$\left. \frac{1}{3}\overline{r}_2 + \frac{1}{3}\overline{r}_3 \mid^{-1} \right] \cdot$$

$$\exp(i\overline{K}\cdot(\overline{\tau}_2 - \overline{\tau}_1))d\overline{\tau}_1 \, d\overline{\tau}_2 \, d\overline{r}_1 \, d\overline{r}_2 \, d\overline{r}_3 \qquad (106)$$

The integration over $\overline{\tau}_2$ space is accomplished using the identify

$$\int \frac{\exp(i\overline{K}\cdot\overline{\tau})}{\mid \overline{r} - \overline{\tau} \mid} d\overline{\tau} = \frac{4\pi}{K^2} \exp(i\overline{K}\cdot r) \qquad (107)$$

and T_d becomes

$$T_d = \frac{4\pi(2\pi)^{-15/2}}{\sqrt{12} \, K^2} \int \psi_H'^*(N;1)\psi_H'(1s;1)\chi_H'(1s^2;2,3) \cdot$$

$$\{\chi'^*(nl;2,3) + \chi'^*(nl;3,2)\} \cdot$$

$$\left[\exp(i\overline{K}\cdot(- \frac{1}{2}r_1 + \frac{1}{3}\overline{r}_2 + \frac{1}{3}\overline{r}_3)) + \exp(i\overline{K}\cdot(\frac{1}{2}\overline{r}_1 - \right.$$

$$\frac{2}{3}\overline{r}_2 + \frac{1}{3}\overline{r}_3)) +$$

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$$\exp(i\overline{K}\cdot(\tfrac{1}{2}\,\overline{r}_1 + \tfrac{1}{3}\,\overline{r}_2 - \tfrac{2}{3}\,\overline{r}_3)) - \exp(i\overline{k}\cdot(-\tfrac{1}{2}\,\overline{r}_1 -$$

$$\tfrac{2}{3}\,\overline{r}_2 + \tfrac{1}{3}\,\overline{r}_3)) -$$

$$\exp(i\overline{K}\cdot(-\tfrac{1}{2}\,\overline{r}_1 + \tfrac{1}{3}\,\overline{r}_2 - \tfrac{2}{3}\,\overline{r}_3)) - \exp(i\overline{K}\cdot(\tfrac{1}{2}\,\overline{r}_1 -$$

$$\tfrac{2}{3}\,\overline{r}_2 - \tfrac{1}{3}\,\overline{r}_3))\Big] \cdot$$

$$d\overline{\tau}_1\ d\overline{r}_1\ d\overline{r}_2\ d\overline{r}_3 \tag{108}$$

Because of the volume normalization of plane waves the integration of $\overline{\tau}_1$ is

$$\int d\overline{\tau}_1 = (2\pi)^3 \tag{109}$$

Performing this integration and factoring terms Equation 108 becomes

$$T_d = \frac{4\pi(2\pi)^{-\frac{9}{2}}}{\sqrt{12}\ K^2} \int \psi_H^{'*}(N;1)\psi_H^{'}(1s;1)\ \cdot$$

$$\{\exp(-\tfrac{i}{2}\,\overline{K}\cdot\overline{r}_1) - \exp(\tfrac{i}{2}\,\overline{K}\cdot\overline{r}_1)\}d\overline{r}_1\ \cdot$$

$$\{\chi_H^{'*}(nl;2,3) + \chi_H^{'*}(nl;3,2)\}\ \cdot\ \chi_H^{'}(1s^2;2,3)\ \cdot$$

$$\exp(i\overline{K}\cdot\tfrac{1}{3}(\overline{r}_2 + \overline{r}_3)) - 2\{\exp(i\overline{K}\cdot(-\tfrac{2}{3}\,r_2 + \tfrac{1}{3}\,\overline{r}_3))\}\ \cdot$$

$$d\overline{r}_2\ d\overline{r}_3 \tag{110}$$

The factor of 2 in the second integral is due to the interchangability of $\overline{r}_2$ and $\overline{r}_3$ before and after the collision.

The form factor of the hydrogen atom in a ground state excited to its Nth excited level is performed in Landau and Lifshitz (Ref 12:578). The second integral is analytically done for simple initial wave functions. If the final state is 1s then

$$\int \exp(-\gamma r)\, \exp(i\overline{K}\cdot\overline{r}) \cdot \frac{1}{2\sqrt{\pi}} \exp(-r)\, d\overline{r} =$$
$$8\sqrt{\pi}\ (\gamma+1)/((\gamma+1)^2 + K^2)^2 \tag{111a}$$

and if the final state is 2s,

$$\int \exp(-\gamma r)\, \exp(i\overline{K}\cdot\overline{r})\, (32\pi)^{-\frac{1}{2}}(2-r)\, \exp(-r/2)d\overline{r} =$$
$$\sqrt{2\pi}\ \frac{(6(\gamma + \tfrac{1}{2})^3 - 3(\gamma + \tfrac{1}{2})^2 + (2\cdot\gamma + 2)K^2)}{((\gamma + \tfrac{1}{2})^2 + K^2)^3} \tag{111b}$$

Using these results, the integration of Equation 110 is easily performed, and

$$T_d = \frac{2(2\pi)^{-\frac{9}{2}}}{\sqrt{3}\ K^2} \int \psi_H'^*(N;1)\{\exp(-i\overline{K}\cdot\tfrac{1}{2}\overline{r}_1) - \exp(i\overline{K}\cdot\tfrac{1}{2}\overline{r}_1)\}\cdot$$

$$\psi_H'(1s;1)\ d\overline{r}\ \cdot$$

$$\Big[F(nl,\alpha+1,\tfrac{1}{3}\overline{K} + \tfrac{\epsilon-1}{3(1+2\epsilon)}\overline{k}_- + \tfrac{1}{3}\overline{k}_e - \tfrac{2\epsilon-1}{3(1+\epsilon)}\overline{k}_H)\ \cdot$$

$$F(1s,\beta,\tfrac{1}{3}\overline{K} + \tfrac{\epsilon-1}{3(1+2\epsilon)}\overline{k}_- + \tfrac{1}{3}\overline{k}_H - \tfrac{2}{3}\overline{k}_e)\ +$$

$$F(nl,\beta+1,\tfrac{1}{3},\overline{K} + \tfrac{\epsilon-1}{3(1+2\epsilon)}\overline{k}_- + \tfrac{1}{3}\overline{k}_e - \tfrac{2\epsilon-1}{3(1+\epsilon)}\overline{k}_H)\ \cdot$$

$$F(1s,\alpha,\tfrac{1}{3}\overline{K} + \tfrac{\epsilon-1}{3(1+2\epsilon)}\overline{k}_- + \tfrac{1}{3}\overline{k}_H - \tfrac{2}{3}\overline{k}_e)\ -$$

$$F(nl,\alpha+1, -\tfrac{2}{3}\overline{K} + \tfrac{\epsilon-1}{3(1+2\epsilon)}\overline{k}_- + \tfrac{1}{3}\overline{k}_e - \tfrac{2\epsilon-1}{3(1+\epsilon)}k_H)\ \cdot$$

$$F(1s,\beta,\tfrac{1}{3},\overline{K} + \tfrac{\epsilon-1}{3(1+2\epsilon)}\overline{k}_- + \tfrac{1}{3}\overline{k}_H - \tfrac{2}{3}\overline{k}_e)\ -$$

$$F(nl,\beta+1, -\tfrac{2}{3}\overline{K} + \tfrac{\epsilon-1}{3(1+2\epsilon)}\overline{k}_- + \tfrac{1}{3}\overline{k}_e - \tfrac{2\epsilon-1}{3(1+\epsilon)}\overline{k}_H)\ \cdot$$

$$F(1s,\alpha,\tfrac{1}{3}\overline{K} + \tfrac{\epsilon-1}{3(1+2\epsilon)}\overline{k}_- + \tfrac{1}{3}\overline{k}_H - \tfrac{2}{3}\overline{k}_e)\ -$$

$$F(nl,\alpha+1,\tfrac{1}{3}\overline{K} + \tfrac{\epsilon-1}{3(1+2\epsilon)}\overline{k}_- + \tfrac{1}{3}\overline{k}_H - \tfrac{2}{3}\overline{k}_e)\ \cdot$$

$$F(1s,\beta, -\tfrac{2}{3}\overline{K} + \tfrac{\epsilon-1}{3(1+2\epsilon)}\overline{k}_- + \tfrac{1}{3}\overline{k}_e - \tfrac{2\epsilon-1}{3(1+\epsilon)}\overline{k}_H)\ -$$

$$F(nl,\beta+1,\tfrac{1}{3}\,\overline{K} + \frac{\epsilon-1}{3(1+2\epsilon)}\,\overline{k}_- + \tfrac{1}{3}\,\overline{k}_H - \tfrac{2}{3}\,\overline{k}_e)\ \cdot$$

$$\left. F(1s,\alpha,-\tfrac{2}{3}\,\overline{K} + \frac{\epsilon-1}{3(1+2\epsilon)}\,\overline{k}_- + \tfrac{1}{3}\,\overline{k}_e - \frac{2\epsilon-1}{3(1+\epsilon)}\,\overline{k}_H)) \right] \quad (112)$$

where the function $F(nl,A,\overline{K})$ is defined as

$$F(1s,A,\overline{K}) = \frac{8\sqrt{\pi}\ (A+1)}{((A+1)^2 + K^2)^2}$$

if $nl = 1s$ and

$$F(2s,\gamma,\overline{K}) = \frac{\sqrt{2\pi}\ \ 6(\gamma + \tfrac{1}{2})^3 - 3(\gamma + \tfrac{1}{2})^2 + (2\gamma + 2\underline{\ }K^2}{\{(\gamma + \tfrac{1}{2})^2 + K^2\}^3}$$

if $nl = 2s$.

Exchange Matrix for the Exchange of Electrons Between H Atoms, $T_{e,H}$

The scattering matrix associated with the exchange of electrons between the H atoms is given by

$$T_{e,H} = \frac{1}{\sqrt{12}}\int \psi_H^*(N;2,1)\psi_R^*(nl;1,2)\psi_e^*(3)\cdot V\cdot$$

$$\psi_H-(1s;2,3)\psi_H(1s;1)d\overline{\tau}\ +$$

$$\frac{1}{\sqrt{12}}\int \psi_H^*(N;3,1)\psi_R^*(nl;1,2)\psi_e^*(2)\cdot V\cdot$$

$$\psi_H-(1s^2;2,3)\psi_H(1s;1)d\overline{\tau} \qquad (113)$$

where $\psi_H^*(N;i,\alpha)$, $\psi_R^*(nl;j,\beta)$, $\psi_e^*(k)$, $\psi_H-(1s^2;2,3)$ and $\psi_H(1s:1)$ are defined in Equations 77, 78 or 79, 80, 75 and 74, respectively. The potential V is different than Equation 72 on the scattering potential in the direct scattering matrix, T_d. The scattering potential for exchange of particles is the electrostatic potential between the two particles. This result is proved by Goldberger and Watson (Ref 9:156-8) and will not be presented here. Therefore the potential for the

exchange of electron 1 and electron 3 is

$$V = V_{13} = |\overline{X}_1 - \overline{X}_3|^{-1} \tag{114}$$

and for the exchange of electron 1 and electron 2 is

$$V = V_{12} = |\overline{X}_1 - \overline{X}_2|^{-1} \tag{115}$$

Therefore $T_{e,H}$ can be written as

$$T_{e,H} = \frac{1}{\sqrt{12}} \int \psi_H^*(N;2,1) \psi_R^*(nl;1,2) \psi_e^*(3) \cdot V_{12} \cdot$$

$$\psi_H(1s;1) \psi_{H^-}(1s^2;2,3) d\overline{\tau} + \cdot$$

$$\frac{1}{\sqrt{12}} \int \psi_H^*(N;3,1) \psi_R^*(nl;1,2) \psi_e^*(2) \cdot V_{13} \cdot$$

$$\psi_H(1s;1) \psi_{H^-}(1s^2;2,3) d\overline{\tau} \tag{116}$$

Because of the indistinguishability of the electrons the two integrals in Equation 116 are equal, therefore $T_{e,H}$ is just double the value of one of the integrals or

$$T_{e,H} = \frac{1}{\sqrt{3}} \int \psi_H^*(N;3,1) \psi_{H^-}^*(nl;1,2) \psi_e^*(2) \cdot V_{13} \cdot$$

$$\psi_H(1s;1) \psi_{H^-}(1s^2;2,3) d\overline{\tau} \tag{117}$$

Using the notation developed in the previous section, specifically Equations 97, 98 and 99, $T_{e,H}$ can be written as

$$T_{e,H} = \frac{(2\pi)^{-15/2}}{\sqrt{3}} \int \psi_H^*(N;3) \psi_H(1s;1) \chi_{H^-}(1s^2;2,3) \chi^*(nl;1) \cdot$$

$$\exp(i\{\overline{k}_- \cdot (\overline{R}_- - \overline{R}_o) - i\overline{k}_H \cdot (\overline{R}_H - \overline{R}_o') -$$

$$i\overline{k}_e(\overline{r}_e - \overline{R}_o')\}) \cdot$$

$$V_{13} \, d\overline{\tau} \tag{118}$$

A change of variables is performed using the transformation matrices

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developed in Appendix A for this exchange. Equation 118 is now

$$T_{e,H} = \frac{(2\pi)^{-15/2}}{\sqrt{3}} \int \psi_H^*(N;3)\psi_H(1s;1)\chi_{H^-}(1s^2;2,3)\chi^*(nl;1)$$

$$\exp(i\{\overline{k}_- \cdot (-\frac{\epsilon}{1+\epsilon}\,\overline{r}_1 + \overline{r}_1' + \frac{\epsilon}{1+2\epsilon}\,\overline{r}_2 - \frac{1+\epsilon}{1+2\epsilon}\,\overline{r}_3) -$$

$$\overline{k}_H \cdot (\frac{\epsilon}{1+\epsilon}\,\overline{r}_1 + \frac{1-\epsilon}{1+\epsilon}\,\overline{r}_1' - \frac{1}{1+\epsilon}\,\overline{r}_3) -$$

$$\overline{k}_e \cdot (\overline{r}_1' + \overline{r}_2 - \overline{r}_3)\}) \cdot$$

$$|\overline{r}_1 - \overline{r}_3|^{-1}\; d\overline{r}_1 d\overline{r}_1' d\overline{r}_2 d\overline{r}_3 d\overline{\tau} \qquad (119)$$

The integration over $\overline{r}_2$ and $\overline{\tau}$-spaces can be done analytically for simple wave functions. The integration of the $\overline{r}_1, \overline{r}_1'$ and $\overline{r}_3'$ can not be done analytically because the resultant wave function orbital coordinates, $\overline{r}_H$, depends upon $\overline{r}_1$, $\overline{r}_2'$ and $\overline{r}_3$, that is the term $\exp(-|-\overline{r}_1 + \overline{r}_1' - \overline{r}_3|)$ appears in the integrand. Because of this problem, the effect of the exchange of electrons can not be seen in the differential cross section, because this integral can not be performed analytically. Further discussions on this matrix is presented later in the Conclusions and Recommendations section.

Exchange Matrix for the Exchange of Electrons Between the Target H Atom and the Free Electron, $T_{e,f}$

The scattering matrix associated with the exchange of electrons between the target H atom and the free electron is given by

$$T_{e,f} = \frac{1}{\sqrt{12}} \int \psi_H^*(N;2,1)\psi_R^*(nl;3,2)\psi_e^*(1)\cdot V\cdot$$

$$\psi_H(1s;1)\psi_{H^-}(1s^2;2,3)d\overline{\tau} +$$

$$\frac{1}{\sqrt{12}} \int \psi_H^*(N;3,1)\psi_R^*(nl;3,2)\psi_e^*(1)\cdot V\cdot$$

$$\psi_H(1s;1)\psi_{H^-}(1s^2;2,3)d\overline{\tau} \qquad (120)$$

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where $\psi_H^*(N;i,\alpha)$, $\psi_R^*(nl;j,\beta)$, $\psi_e^*(k)$, $\psi_{H^-}(1s^2;2,3)$ and $\psi_H(1s;1)$ are defined in Equations 77, 78 or 79, 80, 75 and 74, respectively. The potential is, following the convention presented in the previous chapter, V_{12} or V_{13} depending upon the particles exchanged. Once again the electrons 2 and 3 are interchangable, therefore

$$T_{e,f} = \frac{(2\pi)^{-15/2}}{\sqrt{3}} \int \psi_H^*(N;2)\psi_H(1s;1)\chi_{H^-}(1s^2;2,3)\chi^*(nl;3) \cdot$$

$$\exp\{i(\overline{k}_- \cdot (\overline{R}_- - \overline{R}_o) - \overline{k}_H \cdot (\overline{R}_H - \overline{R}_o') - \overline{k}_e \cdot (\overline{r}_e - \overline{R}_o'))\} \cdot$$

$$|\overline{X}_1 - \overline{X}_2|^{-1} \cdot d\overline{\tau} \qquad (121)$$

where $\psi_H^*(N;2)$, $\psi_H(1s;1)$, $\chi_{H^-}(1s^2;2,3)$ and $\chi^*(nl;3)$ are defined following the notation in Equations 97, 98, 99 and 96b, respectively. A change of variables is performed using the transformation matrices developed in Appendix A for this exchange. Equation 121 is now written as

$$T_{e,f} = \frac{(2\pi)^{-15/2}}{\sqrt{3}} \int \psi_H^*(N,2)\psi_H(1s,1) \ \chi_{H^-}(1s^2;2,3)\chi^*(nl,3) \cdot$$

$$\exp\{i(\overline{k}_- \cdot (-\frac{\epsilon}{1+\epsilon}\overline{r}_1 + \overline{r}_1' - \frac{1+\epsilon}{1+2\epsilon}\overline{r}_2 + \frac{\epsilon}{1+2\epsilon}\overline{r}_3) -$$

$$\overline{k}_H \cdot (\frac{1}{1+\epsilon}\overline{r}_1' - \overline{r}_2 + \frac{\epsilon}{1+\epsilon}\overline{r}_3) -$$

$$\overline{k}_e \cdot (\frac{1}{1+\epsilon}\overline{r}_1'))\} \cdot |\overline{r}_1 - \overline{r}_1'|^{-1} d\overline{\tau}d\overline{r}_1 d\overline{r}_1'd\overline{r}_2 d\overline{r}_3$$

$$(122)$$

The integration over $\overline{\tau}$, $\overline{r}_2$ and $\overline{r}_3$ space can be done analytically for a simple H^- wave function. However there is an integral of the form

$$\int \psi_H^*(N;2)\psi_H(1s,1)\exp(i\ \overline{r}_1 \cdot (-\frac{\epsilon}{1+\epsilon}\overline{k}_-)) \cdot$$

$$\exp(i\ \overline{r}_1' \cdot (\overline{k}_- - \frac{1}{1+\epsilon}(\overline{k}_H + \overline{k}_e))) \cdot |\overline{r}_1 - \overline{r}_1'|^{-1} \cdot d\overline{r}_1 d\overline{r}_1'$$

$$(123)$$

This can not be done analytically and therefore the effect of exchange of electrons can not be included unless a numerical integration of the

spatial coordinates is done. A further discussion of this scattering matrix is presented in the Conclusion and Recommendation sections.

Exchange Matrix for Exchange of Protons Between the H Atoms, T_p

The scattering matrix associated with the exchange of protons between the H atoms is given by

$$T_p = \frac{1}{\sqrt{12}} \int \psi_H^*(N;1,2)\psi_R^*(nl;2,1)\psi_e^*(3) \cdot V_p \cdot$$
$$\psi_{H^-}(1s^2;2,3)\psi_H(1s;1) \; d\bar{\tau} \; +$$
$$\frac{1}{\sqrt{12}} \int \psi_H^*(N;1,2)\psi_R^*(nl:3,1)\psi_e^*(2) \cdot V_p \cdot$$
$$\psi_{H^-}(1s^2;2,3)\psi_H(1s;1) \; d\bar{\tau} \tag{124}$$

The same notation has been used here that was used in the previous three sections. Performing the change of variables and rewriting the wavefunctions using Equations 97, 98 and 99, Equation 124 can be re-written as

$$T_p = \frac{(2\pi)^{-15/2}}{\sqrt{3}} \int \psi_H^*(N;1)\psi_H(1s;1)\chi^*(nl;3)\chi_{H^-}(1s^2;2,3) \; \cdot$$
$$\exp\{i(\bar{k}_- \cdot (-\frac{1}{1+\epsilon}\bar{r}_1 - \bar{r}_1' + \frac{\epsilon}{1+2\epsilon}\bar{r}_2 + \frac{\epsilon}{1+2\epsilon}\bar{r}_3) -$$
$$\bar{k}_H \cdot (-\frac{1}{1+\epsilon}\bar{r}_1 + \frac{1-\epsilon}{1+\epsilon}\bar{r}_1' + \frac{\epsilon}{1+\epsilon}\bar{r}_3) -$$
$$\bar{k}_e \cdot (-\frac{\epsilon}{1+\epsilon}\bar{r}_1' + \bar{r}_2))\} \cdot |\bar{r}_1 - \bar{r}_1'|^{-1} \cdot$$
$$d\bar{\tau} \; d\bar{r}_1 \; d\bar{r}_2 \; d\bar{r}_3 \; d\bar{r}_1' \; . \tag{125}$$

The integration of $\bar{\tau}$ and $\bar{r}_2$ can be done analytically, but once again $r_H = |\bar{r}_1 - \bar{r}_1' + \bar{r}_3|$ and with this term in the resultant H atom wave-function the integration must be done numerically.

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Exchange Matrix for Exchange of H Atoms, T_H

The scattering matrix associated with the exchange of H atoms between the final H atoms is given by

$$T_d = \frac{1}{\sqrt{12}} \int \psi_H^*(N;2,2)\psi_R^*(nl;1,1)\psi_e^*(3) \cdot \{ V_{12} + V_p \} \cdot$$

$$\psi_H(1s;1)\psi_{H^-}(1s^2;2,3)d\bar{\tau} +$$

$$\frac{1}{\sqrt{12}} \int \psi_H(N;3,2)\psi_R^*(nl;1,1)\psi_e^*(2) \cdot \{ V_{13} + V_p \} \cdot$$

$$\psi_H(1s;1)\psi_{H^-}(1s^2;2,3)d\bar{\tau} \tag{126}$$

The same notation has been used that was previously used in the preceeding sections. Performing the change of variables and rewriting the wavefunctions following the format of Equations 97, 98 and 99 Equation 126 becomes

$$T_H = \frac{(2\pi)^{-15/2}}{\sqrt{3}} \int \psi_H^*(N;3)\psi_H(1s;1)\chi^*(nl;1)\chi_{H^-}(1s^2;2,3) \cdot$$

$$\exp\{i(\bar{k}_- \cdot (\bar{\tau}_2 - \bar{\tau}_1 + \frac{\epsilon-1}{3(1+2\epsilon)}(\bar{r}_2 + \bar{r}_3) - \frac{\epsilon-1}{2(1+\epsilon)}\bar{r}_1) -$$

$$\bar{k}_H \cdot (\bar{\tau}_1 - \bar{\tau}_2 + \frac{\epsilon-1}{2(1+\epsilon)}\bar{r}_1 + \frac{1}{3}\bar{r}_2 - \frac{2\epsilon-1}{3(1+\epsilon)}\bar{r}_3) -$$

$$\bar{k}_e \cdot (\bar{r}_2 - \frac{\epsilon}{1+\epsilon}\bar{r}_3))\} \cdot \left[|\bar{\tau}_1 - \bar{\tau}_2 + \frac{1}{2}\bar{r}_1 + \right.$$

$$\frac{1}{3}\bar{r}_2 - \frac{2}{3}\bar{r}_3|^{-1} +$$

$$\left. |\bar{\tau}_1 - \bar{\tau}_2 - \frac{1}{2}\bar{r}_1 + \frac{1}{3}(\bar{r}_2 + \bar{r}_3)|^{-1} \right]$$

$$d\bar{r}_1 \, d\bar{r}_2 \, d\bar{r}_3 \, d\bar{\tau}_1 \, d\bar{\tau}_2 \tag{127}$$

Performing the integration of $\bar{\tau}_2$ and $\bar{\tau}_1$ space, using Equations 107 and 109, respectively, gives

$$T_H = \frac{4\pi(2\pi)^{-9/2}}{(\overline{k}_- + \overline{k}_H)^2\sqrt{3}} \int \psi_H^*(N;3)\psi_H(1s;1)\chi^*(nl;1)\chi_{H^-}(1s^2;2,3) \cdot$$

$$\exp\{i(\overline{k}_- \cdot (\frac{\epsilon-1}{3(1+2\epsilon)}\,(\overline{r}_2 + \overline{r}_3) - \frac{\epsilon-1}{2(1+\epsilon)}\,\overline{r}_1) -$$

$$\overline{k}_H \cdot (\frac{\epsilon-1}{2(1+\epsilon)}\,\overline{r}_1 + \frac{1}{3}\,\overline{r}_2 - \frac{2\epsilon-1}{3(1+\epsilon)}\,\overline{r}_3) -$$

$$\overline{k}_e \cdot (\overline{r}_2 - \frac{\epsilon}{1+\epsilon}\,\overline{r}_3))\} \cdot$$

$$\{\exp(i(\overline{k}_- + \overline{k}_H) \cdot (\frac{1}{2}\,\overline{r}_1 + \frac{1}{3}\,\overline{r}_2 - \frac{2}{3}\,\overline{r}_3)) +$$

$$\exp(i(\overline{k}_- + \overline{k}_H) \cdot (-\frac{1}{2}\,\overline{r}_1 + \frac{1}{3}\,\overline{r}_2 + \frac{1}{3}\,\overline{r}_3))\} \cdot$$

$$d\overline{r}_1\ d\overline{r}_2\ d\overline{r}_3 \tag{128}$$

This scattering matrix is proportional to $(\overline{k}_- + \overline{k}_H)^{-2}$ which is much smaller than $(\overline{k}_- - \overline{k}_H - \overline{k}_e)^{-2}$ which is what the direct scattering matrix is proportional to. Therefore at the large energies of the incoming H^- ion, the exchange of H atoms can be ignored.

Exchange Matrix for Exchange of Protons Between H Atoms and Exchange of Electrons Between the Target Atom and Free Electron, $T_{p,f}$

The scattering matrix associated with the exchange of protons between the final H atoms and the exchange of electrons between the final target H atom and the free electron is given by

$$T_{p,f} = \frac{1}{\sqrt{12}} \int \psi_H^*(N;2,2)\psi_{H^-}^*(nl;3,1)\psi_e^*(1) \cdot \{V_{12} + V_p\} \cdot$$

$$\psi_H(1s;1)\psi_{H^-}(1s^2;2,3)\ d\overline{\tau} +$$

$$\frac{1}{\sqrt{12}} \int \psi_H^*(N;3,2)\psi_{H^-}^*(nl;2,1)\psi_e^*(1) \cdot \{V_{13} + V_p\} \cdot$$

$$\psi_H(1s;1)\psi_{H^-}(1s^2;2,3)\ d\overline{\tau} . \tag{129}$$

The same notation has been used that was used in the previous five

sections. Performing the change of variables and rewriting the wave-functions following the format of Equations 97, 98 and 99, Equation 129 can be written as

$$T_{p,f} = \frac{(2\pi)^{-15/2}}{\sqrt{3}} \int \psi_H^*(N;3)\psi_H(1s;1)\chi^*(nl;2)\chi_{H^-}(1s^2;2,3) \cdot$$

$$\exp\{i(\overline{k}_- \cdot (-\frac{\epsilon}{1+\epsilon}\overline{r}_1 + \overline{r}_H + \frac{\epsilon}{1+2\epsilon}\overline{r}_2 - \frac{1+\epsilon}{1+2\epsilon}\overline{r}_3) -$$

$$\overline{k}_H \cdot (-\frac{1}{1+\epsilon}\overline{r}_H - \frac{\epsilon}{1+\epsilon}\overline{r}_2 + \overline{r}_3) -$$

$$\overline{k}_e \cdot (\overline{r}_1 - \overline{r}_H - \frac{\epsilon}{1+\epsilon}\overline{r}_2 + \overline{r}_3))\} \cdot$$

$$\{|\overline{r}_1 - \overline{r}_H|^{-1} + |\overline{r}_H - \overline{r}_3|^{-1}\}d\overline{r}_1 \ d\overline{r}_H \ d\overline{r}_2 \ d\overline{r}_3 \ d\tau \qquad (130)$$

Again this integration can not be done analytically. How this affects the total scattering matrix, T_{fi}, is unknown because there is no way to get a handle on the size or properties of this integral.

Summary

Of the six basic scattering matrices, only two can be evaluated analytically. The scattering matrix for the exchange of H atoms was shown to be small compared to the direct scattering matrix. The remaining four scattering matrices can not be evaluated analytically and hence their contributions to the differential cross section are unknown. Because of the high initial energy of the incoming H^- ion, it would be possible to assume that the contribution of the remaining four scattering matrices to small. Following up on this assumption, the total scattering matrix is then

$$|T_{fi}| = 2|T_d| \qquad (131)$$

In order to prove the validity of the assumption, the four remaining

integrals must be done. Using Equation 131 the differential and total cross section must be found using numerical integration techniques. A discussion of the numerical integration technique is discussed in Appendix B.

V. Results, Conclusions and Recommendations

The purpose of this chapter is to present the results of the
computer program, discuss the results and then recommend further work
that should be done. The computer program, Appendix B, was used to
calculate the differential cross sections for different cases. These
results are discussed and specific conclusions are drawn. Finally
there are some recommendations concerning further work in this field.

Results

The differential cross section was calculated for many different
cases and conditions. The energy for all the cross sections was either
2 MeV or 200 MeV. The factors varied were the ratio of the electron
mass to the proton mass, the target atoms mass and the final states.
Where possible the results in this study are compared to Genoni and
Wright (Ref 8:4). The differential cross section presented is really
$\frac{d\sigma}{d\theta}$, not $\frac{d\sigma}{d\Omega}$. The two are related by

$$\frac{d\sigma}{d\theta} = 2\pi \sin \theta \frac{d\sigma}{d\Omega}$$

Comparisons were made for different incoming energies. Figure 2
and Figure 3 are comparisons of differential cross sections for in-
coming energies of 2 MeV and 200 MeV, respectively. The differential
cross sections calculated in this thesis are designated F(nl), where
nl signifies the final state of the resultant H atom. Those calculated
by Genoni and Wright are designated GW(nl). In both cases there is a
significant difference between the present values and the values from
Genoni and Wright.

There are two basic reasons for the differences in the above
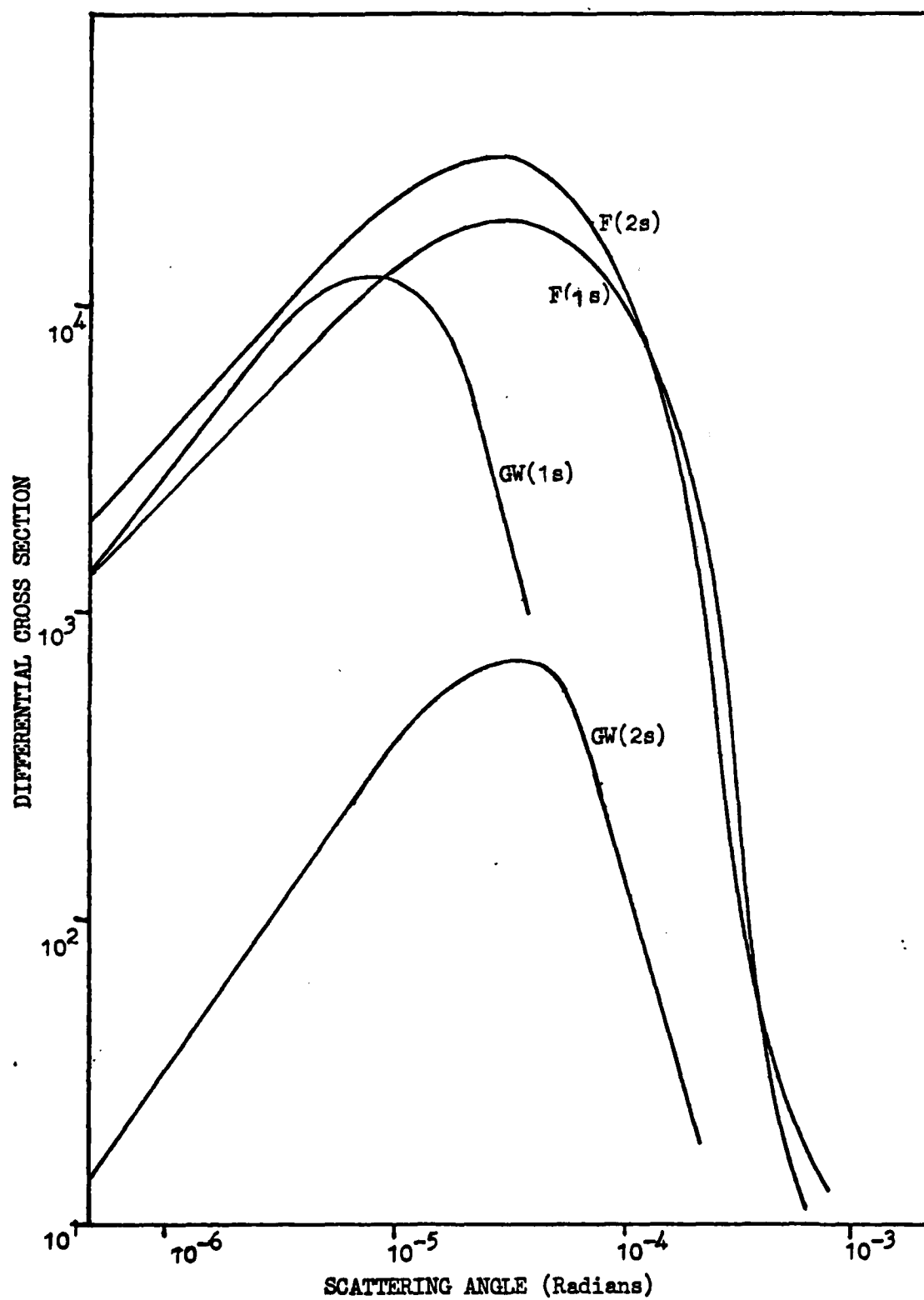cross sections. The first difference is that Genoni and Wright include

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Figure 2. Comparison of Differential Cross Section for 2 MeV
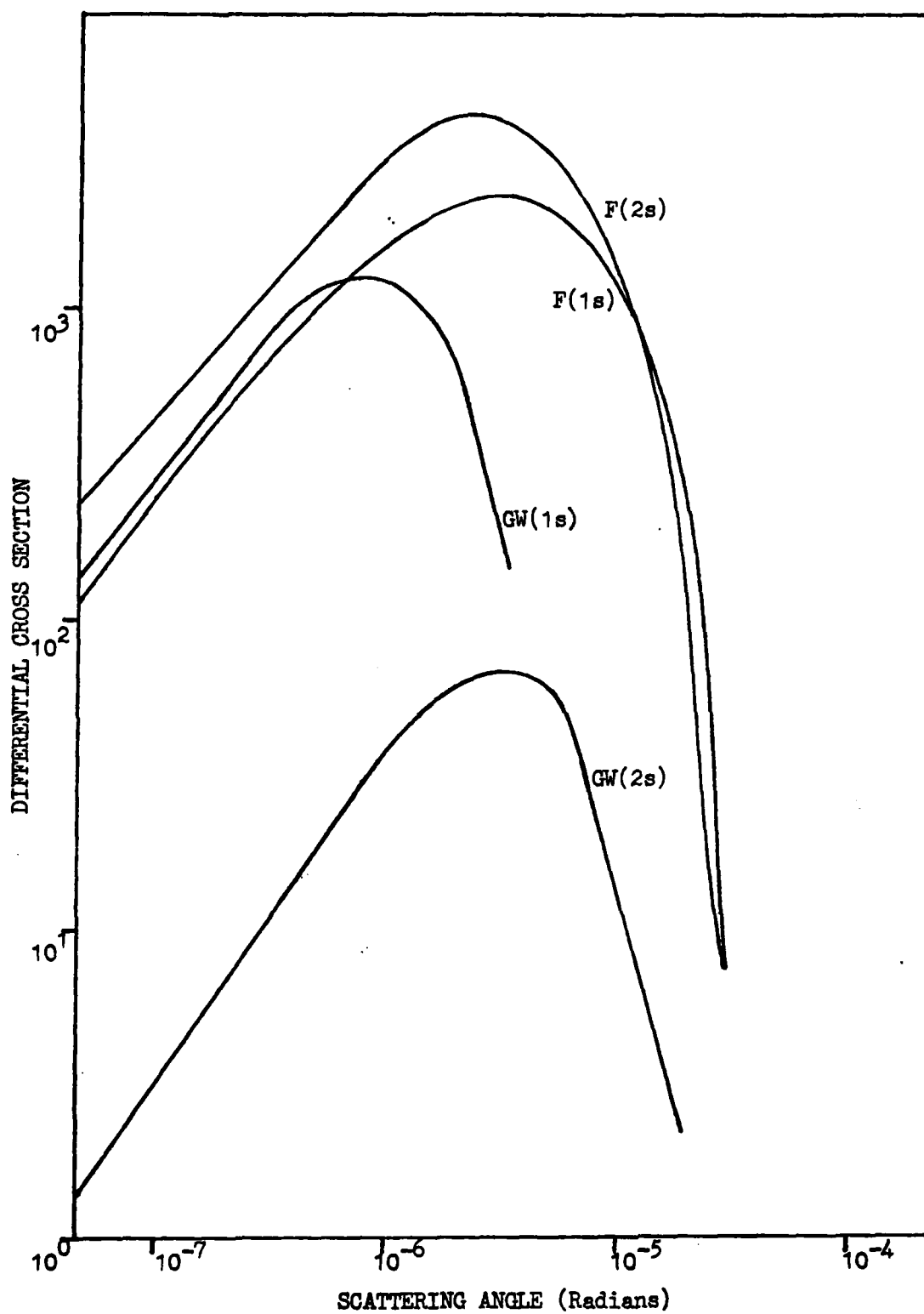
Figure 3. Comparison of Differential Cross Section for 200 MeV

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the differential cross section associated with ionization of the

target H atom and the present value does not. The second difference is

the most important with respect to the magnitude of the differential

cross section. Genoni and Wright have assumed that after the collision

the electron will be in the vicinity of the resultant H atom for an

appreciable amount of time. Because of this assumption, the Hamilton-

ian for the initial H^- ion system and the final $H - e^-$ system is the

same. They then assumed that the final wavefunction must be orthogonal

to the initial H^- ion wavefunction. They orthogonalized according to

the Schmidt orthogonalization procedure or

$$|f\rangle = |\tilde{f}\rangle - \langle i|\tilde{f}\rangle|i\rangle$$

where $|\tilde{f}|$ is the wave function of the $H - e^-$ system and $|i\rangle$ is the H^-

ion wave function. By introducing this type of wave function there is

a major difference because of the subtraction of part of the wave

function. This accounts for the major differences in the compared data.

A minor, as yet to be investigated, effect could possibly be that

Genoni and Wright have assumed that the ratio of the electron's mass

to the proton's mass is zero.

The effect of setting the ratio of the electrons mass to the

protons mass to zero is presented in Figure 4. The ratio ϵ was set

equal to zero for the nl = 1s and 2s and for energies 2 MeV and 200 MeV.

The differential cross section, for $\epsilon = 0$, is designated $F(E, nl, 0)$,

where E is the incoming energy and nl is the final state. When $\epsilon \neq 0$,

the cross section is designated as $F(E, nl)$. It is evident that if

$\epsilon = 0$, there is a significant change of the cross section at 200 MeV.

This is due to the fact that ϵk_- or ϵk_H is approximately equal to the

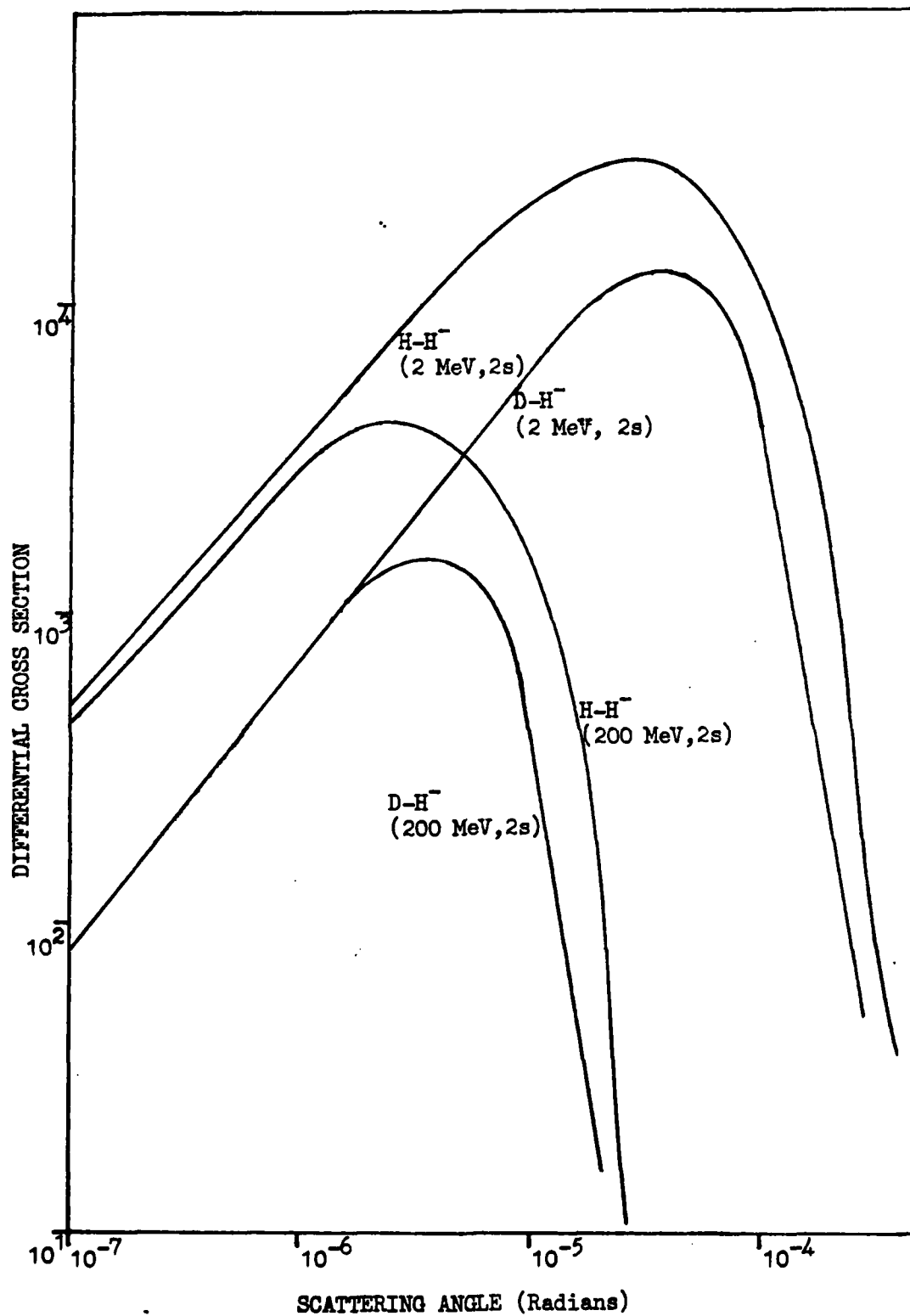electron momentum k_e. Therefore the effect of the ratio ϵ is very

Figure 5. Differential Cross Section for D-H Reaction

significant and must be included in the calculations.

To illustrate the effect of using heavier targets, the differential cross section for nl = 2s was calculated using a target atom that was Deuterium. Because the electron's orbital wave functions depend primarily upon the electrostatic effects, the wavefunctions for deuterium would essentially be the same as those of hydrogen. Therefore hydrogen wavefunctions were used and the mass of the target was $M_T = 3673.104 \, m_e$. Figure 5 illustrates that the added mass has decreased the size of the cross section but has not significantly changed the shape. By increasing the mass of the target atom the overall deflection of the beam can be decreased, assuming a Hartree-Fock wave function for the target atom.

The total cross section is calculated for the H - H$^-$ reaction. Figure 6 compares the value obtained with that obtained by Genoni and Wright. The total cross section is high by an order of magnitude all cases. The reason for this is because of the larger differential cross section obtained in this study.

Conclusions

The results obtained in this study compare in shape but are consistently larger in magnitude with results obtained in earlier work. The main reason for this effect is due to the difference in the formulation of the scattering problem. The effect of exchange could not be included in the results because of the difficulty in obtaining analytic solutions to the integrals involved. This effect could, in theory, change the overall shape and size of the differential cross sections drastically.

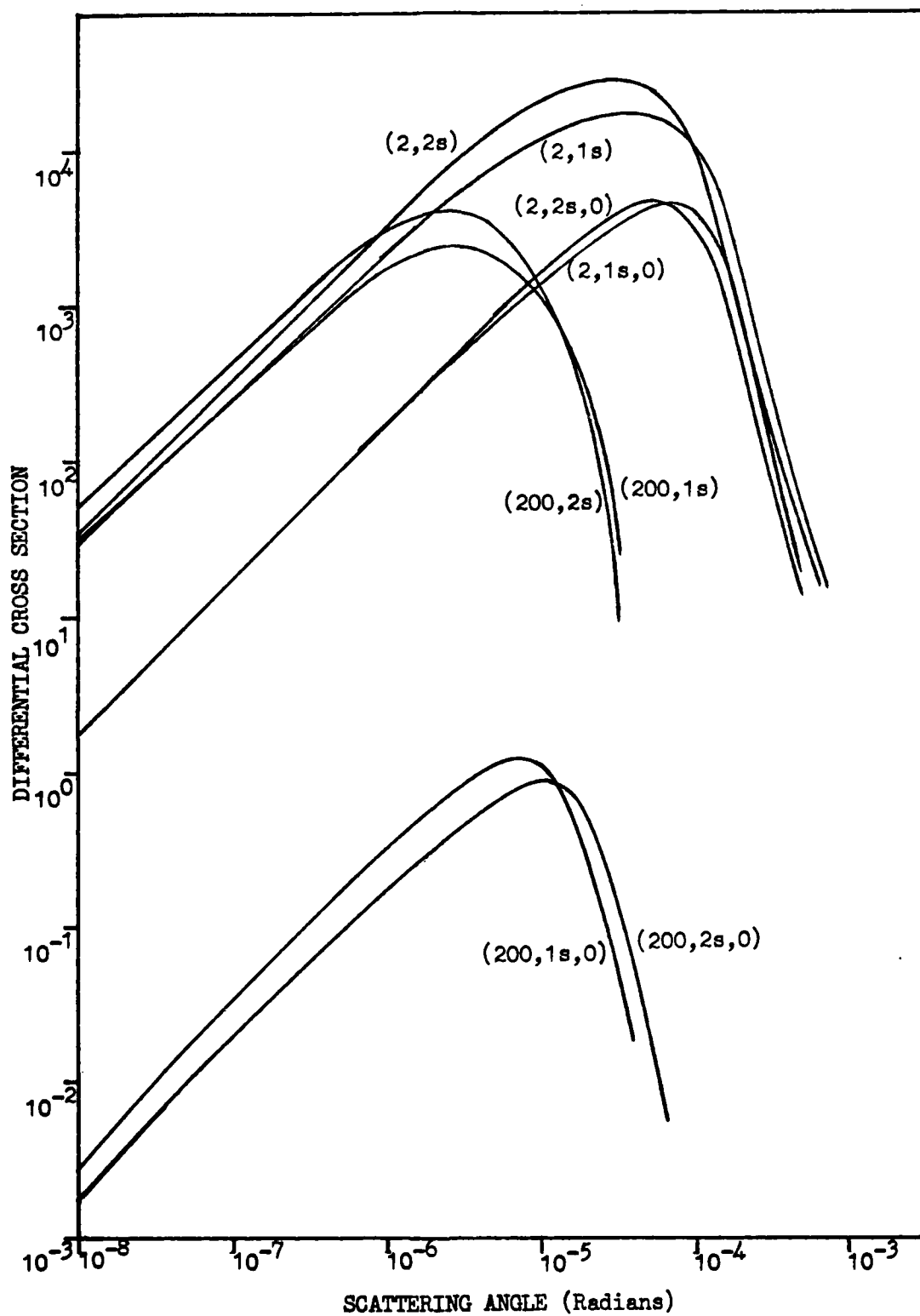The effect of heavier target atoms was investigated using a

44

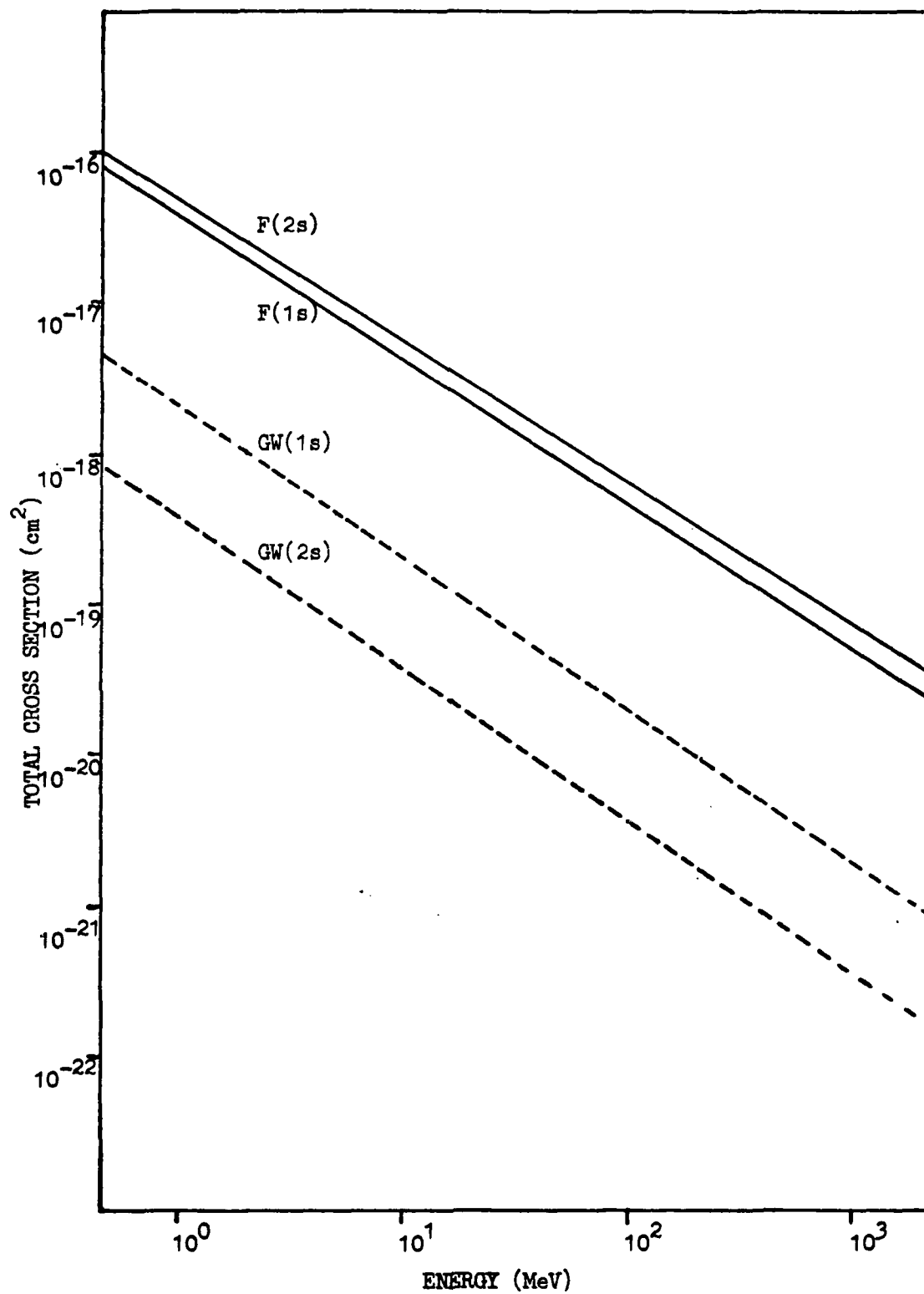Figure 4. Effect of Setting $m_e/M_p = 0$

45

Figure 6. Total Cross Section

deuterium atom instead of hydrogen as a target atom. The increase in mass tended to decrease the size of the cross section, but the shape was essential the same. Further work with different atomic systems is needed.

Finally the total cross section for each final state was larger than that obtained by Genoni and Wright. This was due to the larger and wider differential cross sections calculated in this work.

In summary, it is valid to use the first term of the Born Series to calculate the differential cross section for electron detachment. The incoming energy must be greater than the binding energy or the Born Approximation will need more terms of the Born Series. Special attention is called for in regards to antisymmetrization of the final wave function, and hence exchange.

Recommendations

Some questions have been answered concerning the differential cross section. However, there are still some areas that need to be investigated. There is a need to understand how heavier targets affect the differential cross section. This could be investigated using Hartree-Fock wavefunctions for the target atom and performing the integration of the spatial coordinates numerically.

The exchange scattering matrices need to be evaluated and compared to the direct scattering matrix. By performing the integrations numerically the assumption that the exchange integrals are small, compared to the direct scattering matrix can be investigated. This integration would most probably be done numerically using a Monte-Carlo integration routine.

There should be an investigation into the effect of using better wavefunctions for the H^- ion. Different wavefunctions could be used to see how the differential cross section changes. Once again a Monte-Carlo integration routine would be needed because this calculation would require a 15-fold integration. By combining the above recommendations, a general program could be produced that would use a H^- wavefunction that has been shown to be reasonably accurate, and given an arbitrary target atom, the program could calculate a differential cross section for this system with exchange included.

A final recommendation would be to see if it is possible to sum the Born Series and obtain a better approximation to the scattering potential. This is most probably not a simple task and should only be done if absolutely necessary. An example of when this would be necessary would be when the incoming energy of the H^- ion is very small or on the order of the binding energy of the H system.

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Development of Integration Variables

It is necessary to develop a coordinate system that spans the initial configuration space, the final configuration space and the scattering potential space. A basis set of coordinates are the position vectors of each particle relative to the origin, this basis is designated

$$\overline{Z} = (\overline{X}_1, \overline{R}_1, \overline{X}_2, \overline{X}_3, \overline{R}_3) \tag{A-1}$$

where $\overline{X}_i$ is the position vector of electron i and $\overline{R}_j$ is the position vector of proton j. The general procedure will be done for the case of no exchange of particles, but is easily extended to the cases of exchange.

The initial configuration consists of electron 1 and proton 1 in the target H atom and electron 2 and 3 and proton 2 in the H⁻ ion. This configuration is described completely by the coordinates

$$\overline{Z}_o = (\overline{r}_1, \overline{R}_o, \overline{r}_2, \overline{r}_3, \overline{R}_-) \tag{A-2}$$

where $\overline{r}_i$ is the position vector of the ith electron relative to the proton it is bound to, and $\overline{R}_o$ and $\overline{R}_-$ are the position vectors of the center of mass of the H target atom and H⁻ ion respectively. $\overline{Z}_o$ is written in terms of $\overline{Z}$

$$\overline{Z}_o = \begin{bmatrix} 1 & -1 & & & \\ \dfrac{\epsilon}{1+\epsilon} & \dfrac{1}{1+\epsilon} & & & \\ & & 1 & 0 & -1 \\ & & 0 & 1 & -1 \\ & & \dfrac{\epsilon}{1+2\epsilon} & \dfrac{\epsilon}{1+2\epsilon} & \dfrac{1}{1+2\epsilon} \end{bmatrix} \cdot \overline{Z} \tag{A-3}$$

where ϵ is the ratio of the electrons mass to the protons mass. After the collision electron 2 will be assumed to be in the continuous state and electron 3 will be in the resultant H atom, this system is defined by the coordinates

$$\bar{Z}_o' = (\bar{r}_1', \bar{R}_o', \bar{r}_e, \bar{r}_H, \bar{R}_H) \tag{A-4}$$

where $\bar{r}_e$ is the position vector of the free electron and $\bar{R}_o'$ and $\bar{R}_H$ are the position vectors of the center of mass for the H target atom and resultant H atom, respectively. $\bar{Z}_o'$ written in terms of the $\bar{Z}$ coordinate system is

$$\bar{Z}_o' = \begin{bmatrix} 1 & -1 & & & \\ \dfrac{\epsilon}{1+\epsilon} & \dfrac{1}{1+\epsilon} & & & \\ & & 1 & & \\ & & & 1 & -1 \\ & & & \dfrac{\epsilon}{1+\epsilon} & \dfrac{1}{1+\epsilon} \end{bmatrix} \cdot \bar{Z} \tag{A-5}$$

The orbital wave functions for the H target depends upon the magnitude of the electron position vector relative to the proton to which it is bound. This position vector depends explicitly upon the proton and electron position vectors relative to the origin. It is necessary to remove this dependence in order that the integration be done analytically. The orbital position vectors are

$$\bar{Z}' = \begin{bmatrix} \bar{r}_1 \\ \bar{r}_1' \\ \bar{r}_2 \\ \bar{r}_3 \\ \bar{r}_H \end{bmatrix} = \begin{bmatrix} 1 & -1 & & & \\ 1 & -1 & & & \\ & & 1 & 0 & -1 \\ & & 0 & 1 & -1 \\ & & 0 & 1 & -1 \end{bmatrix} \cdot \bar{Z} \tag{A-6}$$

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Obviously $\bar{r}_1 = \bar{r}_1'$ and $\bar{r}_H = \bar{r}_3$, therefore the above matrix has a rank of 3, and two independent vectors can be chosen that can be used to describe the system. $\bar{\tau}_1$ and $\bar{\tau}_2$ are chosen so that they are orthogonal to $\bar{r}_1$, $\bar{r}_2$ and $\bar{r}_3$ and normalized so that the determinant of the matrix is 1, this gives

$$\bar{Z}' = \begin{bmatrix} \bar{r}_1 \\ \bar{\tau}_1 \\ \bar{r}_2 \\ \bar{r}_3 \\ \bar{\tau}_2 \end{bmatrix} = \begin{bmatrix} 1 & -1 & & & \\ \frac{1}{2} & \frac{1}{2} & & & \\ & & 1 & 0 & -1 \\ & & 0 & 1 & -1 \\ & & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{bmatrix} \cdot \bar{Z} \qquad (A-7)$$

Now $\bar{Z}$ can be written in terms of $\bar{Z}'$ or

$$\bar{Z} = \begin{bmatrix} \bar{X}_1 \\ \bar{R}_1 \\ \bar{X}_2 \\ \bar{X}_3 \\ \bar{R}_2 \end{bmatrix} = \begin{bmatrix} \frac{1}{2} & 1 & & & \\ -\frac{1}{2} & 1 & & & \\ & & \frac{2}{3} & -\frac{1}{3} & 1 \\ & & -\frac{1}{3} & \frac{2}{3} & 1 \\ & & -\frac{1}{3} & -\frac{1}{3} & 1 \end{bmatrix} \cdot \bar{Z}' \qquad (A-8)$$

and writing $\bar{Z}_o$ and $\bar{Z}_o'$ in terms of $\bar{Z}'$, give

$$\bar{Z}_o = \begin{bmatrix} 1 & 0 & & & \\ \frac{\varepsilon-1}{2(1+\varepsilon)} & 1 & & & \\ & & 1 & 0 & 0 \\ & & 0 & 1 & 0 \\ & & \frac{\varepsilon-1}{3(1+2\varepsilon)} & \frac{\varepsilon-1}{3(1+2\varepsilon)} & 1 \end{bmatrix} \cdot \bar{Z}' \qquad (A-9)$$

$$
\bar{Z}_o' = \begin{bmatrix} 1 & 0 & & & \\ \dfrac{\epsilon-1}{2(1+\epsilon)} & 1 & & & \\ & & \dfrac{2}{3} & -\dfrac{1}{3} & 1 \\ & & 0 & 1 & 0 \\ & & -\dfrac{1}{3} & \dfrac{2\epsilon-1}{3(1+\epsilon)} & 1 \end{bmatrix} \cdot \bar{Z}' \qquad \text{(A-10)}
$$

It is now possible to analytically integrate over the $\bar{Z}'$ set.

The same process was used to develop an integration basis set when particles were exchanged. The initial configuration in the $\bar{Z}$ basis set is the same in all cases. The final configuration is presented in the $\bar{Z}$ basis set and the exchange explained. The $\bar{Z}'$ basis set is then presented and finally $\bar{Z}_o$ and $\bar{Z}_o'$ are written in terms of the $\bar{Z}'$ coordinate set for each exchange.

Exchange of Electrons Between H Atoms

$$
\bar{Z}_o' = \begin{bmatrix} 0 & -1 & 0 & 1 & 0 \\ 0 & \dfrac{1}{1+\epsilon} & 0 & \dfrac{\epsilon}{1+\epsilon} & 0 \\ 0 & 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 & 1 \\ \dfrac{\epsilon}{1+\epsilon} & 0 & 0 & 0 & \dfrac{1}{1+\epsilon} \end{bmatrix} \cdot \bar{Z} \qquad \text{(A-11)}
$$

In this exchange electron 1 and proton 2 are in the resultant H atom while electron 3 and proton 1 are in the H target atom with electron 2 free. The transformation matrix is

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$$
\overline{Z} = \begin{bmatrix}
\dfrac{4}{5} & -\dfrac{3}{5} & -\dfrac{1}{5} & \dfrac{2}{5} & -1 \\[6pt]
-\dfrac{1}{5} & -\dfrac{3}{5} & -\dfrac{1}{5} & \dfrac{2}{5} & -1 \\[6pt]
-\dfrac{1}{5} & \dfrac{2}{5} & \dfrac{4}{5} & -\dfrac{3}{5} & -1 \\[6pt]
-\dfrac{1}{5} & \dfrac{2}{5} & -\dfrac{1}{5} & \dfrac{2}{5} & -1 \\[6pt]
-\dfrac{1}{5} & \dfrac{2}{5} & -\dfrac{1}{5} & -\dfrac{3}{5} & -1
\end{bmatrix} \cdot \overline{Z}{}' \qquad (A\text{-}12)
$$

where $\overline{Z}{}' = (\overline{r}_1, \overline{r}_1', \overline{r}_2, \overline{r}_3, \overline{\tau})$. Writing $\overline{Z}_o$ and $\overline{Z}_o'$ in terms of $\overline{Z}{}'$ gives

$$
\overline{Z}_o = \begin{bmatrix}
1 & 0 & 0 & 0 & 0 \\[6pt]
\dfrac{4\epsilon-1}{5(1+\epsilon)} & -\dfrac{3}{5} & -\dfrac{1}{5} & \dfrac{2}{5} & -1 \\[6pt]
0 & 0 & 1 & 0 & 0 \\[6pt]
0 & 0 & 0 & 1 & 0 \\[6pt]
-\dfrac{1}{5} & \dfrac{2}{5} & \dfrac{3\epsilon-1}{5(1+2\epsilon)} & \dfrac{-3-\epsilon}{5(1+2\epsilon)} & -1
\end{bmatrix} \cdot \overline{Z}{}' \qquad (A\text{-}13)
$$

and

$$
\overline{Z}_o' = \begin{bmatrix}
0 & 1 & 0 & 0 & 0 \\[6pt]
-\dfrac{1}{5} & \dfrac{2\epsilon-3}{5(1+\epsilon)} & -\dfrac{1}{5} & \dfrac{2}{5} & -1 \\[6pt]
-\dfrac{1}{5} & \dfrac{2}{5} & \dfrac{4}{5} & -\dfrac{3}{5} & -1 \\[6pt]
-1 & 1 & 0 & -1 & 0 \\[6pt]
\dfrac{4\epsilon-1}{5(1+\epsilon)} & \dfrac{2-3\epsilon}{5(1+\epsilon)} & -\dfrac{1}{5} & \dfrac{2\epsilon-3}{5(1+\epsilon)} & -1
\end{bmatrix} \cdot \overline{Z}{}' \qquad (A\text{-}14)
$$

Exchange of Electrons Between Target H Atom and Free Electron

The final configuration is

$$
\begin{bmatrix}
\overline{r}{}' \\[6pt]
\overline{R}_o' \\[6pt]
\overline{r}_e \\[6pt]
\overline{r}_H \\[6pt]
\overline{R}_H
\end{bmatrix} = \begin{bmatrix}
0 & -1 & 1 & 0 & 0 \\[6pt]
0 & \dfrac{1}{1+\epsilon} & \dfrac{\epsilon}{1+\epsilon} & 0 & 0 \\[6pt]
1 & 0 & 0 & 0 & 0 \\[6pt]
0 & 0 & 0 & -1 & 1 \\[6pt]
0 & 0 & 0 & \dfrac{\epsilon}{1+\epsilon} & \dfrac{1}{1+\epsilon}
\end{bmatrix} \cdot \overline{Z} \qquad (A\text{-}15)
$$

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In this exchange electron 2 and electron 1 have exchanged positions, that is electron 1 is free, electron 2 is in the target atom and electron 3 is in the resultant H atom. The transformation matrix is

$$
\bar{Z} = \begin{bmatrix}
\frac{4}{5} & -\frac{3}{5} & \frac{2}{5} & -\frac{1}{5} & -1 \\[4pt]
-\frac{1}{5} & -\frac{3}{5} & \frac{2}{5} & -\frac{1}{5} & -1 \\[4pt]
-\frac{1}{5} & \frac{2}{5} & \frac{2}{5} & -\frac{1}{5} & -1 \\[4pt]
-\frac{1}{5} & \frac{2}{5} & -\frac{3}{5} & \frac{4}{5} & -1 \\[4pt]
-\frac{1}{5} & \frac{2}{5} & -\frac{3}{5} & -\frac{1}{5} & -1
\end{bmatrix} \cdot \bar{Z}' \tag{A-16}
$$

where $\bar{Z}' = (\bar{r}_1, \bar{r}_1', \bar{r}_2, \bar{r}_3, \bar{\tau})$. Writing $\bar{Z}_0$ and $\bar{Z}_0'$ in terms of $\bar{Z}'$ gives

$$
\bar{Z}_0 = \begin{bmatrix}
1 & 0 & 0 & 0 & 0 \\[4pt]
\frac{4\epsilon-1}{5(1+\epsilon)} & -\frac{3}{5} & \frac{2}{5} & -\frac{1}{5} & -1 \\[4pt]
0 & 0 & 1 & 0 & 0 \\[4pt]
0 & 0 & 0 & 1 & 0 \\[4pt]
-\frac{1}{5} & \frac{2}{5} & \frac{-(3+\epsilon)}{5(1+2\epsilon)} & \frac{3\epsilon-1}{5(1+2\epsilon)} & -1
\end{bmatrix} \cdot \bar{Z}' \tag{A-17}
$$

and

$$
\bar{Z}_0' = \begin{bmatrix}
0 & 1 & 0 & 0 & 0 \\[4pt]
-\frac{1}{5} & \frac{2\epsilon-3}{5(1+\epsilon)} & \frac{2}{5} & -\frac{1}{5} & -1 \\[4pt]
-\frac{1}{5} & \frac{2}{5} & \frac{2}{5} & -\frac{1}{5} & -1 \\[4pt]
0 & 0 & 0 & -1 & 0 \\[4pt]
-\frac{1}{5} & \frac{2}{5} & -\frac{3}{5} & \frac{4\epsilon-1}{5(1+\epsilon)} & -1
\end{bmatrix} \cdot \bar{Z}' \tag{A-18}
$$

Exchange of Protons Between H Atoms

The final configuration is given by

$$\overline{Z} = \begin{bmatrix} 1 & 0 & 0 & 0 & -1 \\ \dfrac{1}{1+\epsilon} & 0 & 0 & 0 & \dfrac{1}{1+\epsilon} \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & -1 & 0 \\ 0 & \dfrac{1}{1+\epsilon} & 0 & \dfrac{\epsilon}{1+\epsilon} & 0 \end{bmatrix} \cdot \overline{Z} \qquad (A\text{-}19)$$

In this exchange, proton 1 is in the resultant H atom, proton 2 is in the H target atom and electron 2 is free. There has been no exchange between electron 1 and 3. The transformation matrix is given by

$$\overline{Z} = \begin{bmatrix} \dfrac{1}{5} & \dfrac{3}{5} & -\dfrac{1}{5} & -\dfrac{1}{5} & 1 \\ -\dfrac{4}{5} & \dfrac{3}{5} & -\dfrac{1}{5} & -\dfrac{1}{5} & 1 \\ \dfrac{1}{5} & -\dfrac{2}{5} & \dfrac{4}{5} & -\dfrac{1}{5} & 1 \\ \dfrac{1}{5} & -\dfrac{2}{5} & -\dfrac{1}{5} & \dfrac{4}{5} & 1 \\ \dfrac{1}{5} & -\dfrac{2}{5} & -\dfrac{1}{5} & -\dfrac{1}{5} & 1 \end{bmatrix} \cdot \overline{Z}' \qquad (A\text{-}20)$$

where $\overline{Z}' = (\overline{r}_1, \overline{r}', \overline{r}_2, \overline{r}_3, \overline{\tau})$. Writing $\overline{Z}_o$ and $\overline{Z}_o'$ in terms of $\overline{Z}'$ gives

$$\overline{Z}_o = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ \dfrac{\epsilon-4}{5(1+\epsilon)} & \dfrac{3}{5} & -\dfrac{1}{5} & -\dfrac{1}{5} & 1 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ \dfrac{1}{5} & -\dfrac{2}{5} & \dfrac{3\epsilon-1}{5(1+2\epsilon)} & \dfrac{3\epsilon-1}{5(1+2\epsilon)} & 1 \end{bmatrix} \cdot \overline{Z}' \qquad (A\text{-}21)$$

and

$$\bar{Z}'_o = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ \dfrac{1}{5} & \dfrac{3\epsilon-2}{5(1+\epsilon)} & -\dfrac{1}{5} & -\dfrac{1}{5} & 1 \\ \dfrac{1}{5} & -\dfrac{2}{5} & \dfrac{4}{5} & -\dfrac{1}{5} & 1 \\ -1 & 1 & 0 & -1 & 0 \\ \dfrac{\epsilon-4}{5(1+\epsilon)} & \dfrac{3-2\epsilon}{5(1+\epsilon)} & -\dfrac{1}{5} & \dfrac{4\epsilon-1}{5(1+\epsilon)} & 1 \end{bmatrix} \cdot \bar{Z}' \qquad (A-22)$$

Exchange of H Atoms

The final configuration is given by

$$\bar{Z}'_o = \begin{bmatrix} & & & 1 & -1 \\ & & & \dfrac{\epsilon}{1+\epsilon} & \dfrac{1}{1+\epsilon} \\ & & 1 & & \\ 1 & -1 & & & \\ \dfrac{1}{1+\epsilon} & \dfrac{1}{1+\epsilon} & & & \end{bmatrix} \cdot \bar{Z} \qquad (A-23)$$

In this exchange, proton 2 and electron 3 are in the H target atom, proton 1 and electron 1 are in the resultant H atom and electron 2 is free. The transformation matrix is

$$\bar{Z} = \begin{bmatrix} \dfrac{1}{2} & 1 & & & \\ -\dfrac{1}{2} & 1 & & & \\ & & \dfrac{2}{3} & -\dfrac{1}{3} & 1 \\ & & -\dfrac{1}{3} & \dfrac{2}{3} & 1 \\ & & -\dfrac{1}{3} & -\dfrac{1}{3} & 1 \end{bmatrix} \cdot \bar{Z}' \qquad (A-24)$$

where $\bar{Z}' = (\bar{r}_1, \bar{\tau}_1, \bar{r}_2, \bar{r}_3, \bar{\tau}_2)$. Writing $\bar{Z}_o$ and $\bar{Z}'_o$ in terms of $\bar{Z}'$ gives

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$$\bar{Z}_o = \begin{bmatrix} 1 & 0 & & & \\ \frac{\epsilon-1}{2(1+\epsilon)} & & & & \\ & & 1 & 0 & 0 \\ & & 0 & 1 & 0 \\ & & \frac{\epsilon-1}{3(1+2\epsilon)} & \frac{\epsilon-1}{3(1+2\epsilon)} & 1 \end{bmatrix} \cdot \bar{Z}' \qquad (A\text{-}25)$$

and

$$\bar{Z}_o' = \begin{bmatrix} & & 0 & 1 & 0 \\ & & -\frac{1}{3} & \frac{2\epsilon-1}{3(1+\epsilon)} & 1 \\ & & \frac{2}{3} & -\frac{1}{3} & 1 \\ 1 & 0 & & & \\ \frac{\epsilon-1}{2(1+\epsilon)} & 1 & & & \end{bmatrix} \cdot \bar{Z}' \qquad (A\text{-}26)$$

Exchange of Protons Between H Atoms and Exchange of Electrons Between Target H Atom and Free Electron

The final configuration is given by

$$\bar{Z}_o' = \begin{bmatrix} 0 & 0 & 1 & 0 & -1 \\ 0 & 0 & \frac{\epsilon}{1+\epsilon} & 0 & \frac{1}{1+\epsilon} \\ 1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 1 & 0 \\ 0 & \frac{1}{1+\epsilon} & 0 & \frac{\epsilon}{1+\epsilon} & 0 \end{bmatrix} \cdot \bar{Z} \qquad (A\text{-}27)$$

In this exchange, proton 2 and electron 3 are in the target H atom, proton 1 and electron 2 are in the resultant H atom, and electron 1 is free. The transformation matrix is then

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$$\bar{Z} = \begin{bmatrix} \frac{4}{5} & -\frac{3}{5} & -\frac{1}{5} & \frac{2}{5} & -1 \\ -\frac{1}{5} & -\frac{3}{5} & -\frac{1}{5} & \frac{2}{5} & -1 \\ -\frac{1}{5} & \frac{2}{5} & \frac{4}{5} & -\frac{3}{5} & -1 \\ -\frac{1}{5} & \frac{2}{5} & -\frac{1}{5} & \frac{2}{5} & -1 \\ -\frac{1}{5} & \frac{2}{5} & -\frac{1}{5} & -\frac{3}{5} & -1 \end{bmatrix} \cdot \bar{Z}' \qquad \text{(A-28)}$$

where $\bar{Z}' = (\bar{r}_1, \bar{r}_H, \bar{r}_2, \bar{r}_3, \bar{\tau})$. Writing $\bar{Z}_o$ and $\bar{Z}'_o$ in terms of $\bar{Z}'$ gives

$$\bar{Z}_o = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ \frac{4\epsilon-1}{5(1+\epsilon)} & -\frac{3}{5} & -\frac{1}{5} & \frac{2}{5} & -1 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ -\frac{1}{5} & \frac{2}{5} & \frac{3\epsilon-1}{5(1+2\epsilon)} & \frac{-(3+\epsilon)}{5(1+2\epsilon)} & -1 \end{bmatrix} \cdot \bar{Z}' \qquad \text{(A-29)}$$

and

$$\bar{Z}'_o = \begin{bmatrix} 0 & 0 & 1 & 0 & 0 \\ -\frac{1}{5} & \frac{2}{5} & \frac{4\epsilon-1}{5(1+\epsilon)} & -\frac{3}{5} & -1 \\ \frac{4}{5} & -\frac{3}{5} & -\frac{1}{5} & \frac{2}{5} & -1 \\ 0 & 1 & 0 & 0 & 0 \\ -\frac{1}{5} & \frac{2\epsilon-3}{5(1+\epsilon)} & -\frac{1}{5} & \frac{2}{5} & -1 \end{bmatrix} \cdot \bar{Z}' \qquad \text{(A-30)}$$

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Appendix B

Program to Numerically Integrate the
Differential and Total Cross Sections

Because of the complexity of the terms in the differential and total cross section, the integration over the electron momentum, $\overline{k}_e$, can not be done analytically. A program was written to numerically integrate over the electron momentum, using a Gauss-Legendre integration routine. The magnitude of the electron momentum was integrated over using a 50-point Gauss-Legendre, while the integration over the electron angle was done using a 24-point Gauss-Legendre integration routine.

The incoming energy in the lab frame for the H^- ion, the final states of the H atoms and the scattering angles are inputted to the program. The program then transforms the configuration to the center of mass frame via relativistic mechanics. The Gauss-Legendre integration routine integrates over electron momentum and angle and then transforms the differential cross section to the laboratory frame using

$$\left(\frac{d\sigma}{d\Omega}\right)_{Lab} = \left(\frac{d\sigma}{d\Omega}\right)_{c.m.} \cdot \frac{\left[1 + r^2 + 2r \cos \theta_{cm}\right]^{3/2}}{1 + r \cos \theta_{cm}} \tag{B-1}$$

where $r = V_{cm}/V_f$, V_f is the velocity of the final resultant H atom. The total cross section is then found by using a trapezoid integration over the differential cross section.

The integration routine was tested by comparing the results of the Gauss-Legendre integration to the results computed via Rhomberg integration routine. The results of both integrations agreed to 1 percent. This signifies that either both of the integration routines are wrong or both are right. The probability that both are wrong but give the

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same result is very small, so it can be assumed that the integration routine is correct.

There is no simple analytic solution that can be easily tested using this program. However, each subroutine and function routines were tested with analytic solutions where possible to insure that each was working correctly.

A listing of the program follows. Program MAIN contains all the kinematic transformations and the integration routine. Subroutine FION consists of the integral of the differential cross section. Function FF calculates the atomic form factor for a general excited state N of a hydrogen atom. Function F calculates the atomic form factor for the hydrogen atom transitioning to the 1s or 2s states.

```
      PROGRAM MAIN(INPUT,OUTPUT,TAPE5=OUTPUT,PLOT)
      COMMON/MOM/HKI,SKI,VGM,VI
      COMMON/MASS/HMASS,TMASS,FMASS,RMFH,RMTE,RMTF
      COMMON/CONS/C1,C2,C3,C ,C5,C11,C22,C33,C44,C55
      DIMENSION CHI(60),WEI(60),TIF(30),DIFC(30),DHI(60),DEI(60)
      DIMENSION DTOT(30)
      DATA DTOT/30*0./
      DATA TIF,DIFC,CHI,WEI,CHI,DEI/300*0./
      DATA CHI/.996866,.934031,.985354,.972864,.956611,.936656,.913078
     *,.885908,.855429,.821502,.784556,.744494,.701552,.655896,.607703,
     *.557156,.504456,.449806,.393414,.335500,.276280,.216007,.154691,
     *.0931747,.031098/
      DATA DEI/.00290952,.00675979,.01159005,.01438008,.0181155,
     *.0217802,.0253606,.0286430,.0322137,.0354598,.0365687,.0415284,
     *.0443275,.046355,.049409,.051657,.0537166,.055577,.05/1699,
     *.0586008,.0597051,.0607379,.0614569,.06193F1,.0521766/
      DATA WEI/.0123412233,.0285313886,.0442774368,.0592985849,
     *.0733464614,.0861501615,.0976186521,.1074442701,.1155056681,
     *.1216704729,.1253374563,.1279381353/
      DATA CHI/.995518722,.97672d556,.938274552,.686415527,.820001986,
     *.74012+1516,.648093b519,.545421014,.433793b076,.3154+26797,
     *.1911108675,.0640658920/
      NPOLY=24
      NPOL2=50
      TT1=0.
      C=137.03602585                       $   AU=27.211652
      HMASS=1838.1040+08
      FMASS=1837.10+048
      READ*,ENE       $   READ*,NIST       $   READ*,NHST
      READ*,HKL,HKU,TKL,TKU
      READ*,EPS                            $   READ*, TMASS
      DO 5  I=1,30
      READ*,TIF(I)
      IF(TIF(I).GT.10.0) GO TO 13
    5 CONTINUE
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13 CONTINUE
   I=I-1
   C1=1./(1.+2.*EPS)                                    $ C11=C1*C1
   C2=EPS*C1                                            $ C22=C2*C2
   C3=1./(1.+EPS)                                       $ C33=C3*C3
   C4=EPS*C3                                            $ C44=C4*C4
   C5=C1+C2                                             $ C55=C5*C5
   ENER=ENE
   ENE=ENE/AU
   NP=NPOLY/2
   N2=NFOL2/2
   DO 122 II=1,N2
   DHI(II+N2)=-DHI(II)
122 DEI(II+N2)=DEI(II)
   DO 3 L=1,NP
   CHI(L+NP)=-CHI(L)
3  WEI(L+NP)=WEI(L)
   RMTF=TMASS*FMASS/(TMASS+FMASS)
   RMTH=TMASS*HMASS/(TMASS+HMASS)
   RMTE=TMASS/(1.+TMASS)
   ENT=ENE+(HMASS+TMASS)*C*C
   VI=C*SQRT(1-(HMASS*C*C/(ENE+HMASS*C*C))**2)
   VCM=C*SQRT(ENE**2+2.*ENE*HMASS*C*C)/ENT
   ECM=ENT*SQRT(1-(VCM/C)**2)
   TA=(ECM**2-2.*ECM*HMASS*C*C+(HMASS**2-TMASS**2)*C**4)/(2.*ECM)
   HKI=SQRT(TA*(TA+2.*HMASS*C*C))/C
   SKI=HKI*HKI
   TL1=(TKU+TKL)/2
   TL2=(TKU-TKL)/2
   EL1=(HKU+HKL)/2
   EL2=(HKU-HKL)/2
   DO 20 IG NHST=1,5
   WRITE(5,1) ENER
1  FORMAT(1H1,3X,"THE INCOMING ENERGY IS$ ",1PG12.5)
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      WRITE (5,21) HKL,HKU,TKL,TKU
21    FORMAT(3X,"INTEGRATION RANGE:",/,10X,"ELECTRON MOMENTUM:",
     +F6.3," TO ",F6.3,/,10X,"ELECTRON ANGLE:",F6.3," TO ",F6.3)
      WRITE (5,10) NPOLY,NHST,NIST
10    FORMAT(3X,"NUMBER OF INTEGRATION POINTS PER INTERVAL: ",
     +I5,/,3X,"TARGET FINAL STATE ",I2,5X,"RESULTANT ATOM FINAL STATE ",
     +I1,"S")
      PRINT*,"     GAUSS-LEGENDRE INTEGRATION"
      WRITE (5,11)
11    FORMAT(//,10(1GH+***+*:+**),/,T7,"THETA",T21,"LOG(THETA)",
     +T45,"DIFCR",T54,"LOG(DIFCR)",
     */,10(1GH-+*+*+*:*))
      DIFCS=0.
      DO 30 M=1,30
30    DIFC(M)=0.
      DO 300 J=1,I
      DO 1100 KK=1,NPOL2
      HKE=EL1+EL2*DHI(KK)
      DO 900 KT=1,NPOLY
      TEF=TL1+TL2*CHI(KT)
      CALL FION(HKE,TEF,DIFCF,TIF(J),NIST,NHST)
900   DIFCS=DIFCS+TL2*WEI(KT)*DIFCF
      DIFC(J)=DIFC(J)+EL2*DEI(KK)*DIFCS
1000  DIFCS=0.
      WRITE (5,2) TIF(J),ALOG10(TIF(J)),DIFC(J),ALOG10(DIFC(J))
2     FORMAT(3(1PE15.5,1PE15.5," ::"))
300   CONTINUE
      PRINT*,"..****..***..**..*****..*****.**..*****..***..*.**"
      DO 500 J=1,I
      DTOT(J)=DTOT(J)+DIFC(J)
500   WRITE (5,2) TIF(J),ALOG10(TIF(J)),DTOT(J),ALOG10(DTOT(J))
      TOT=0.
      DO 400 J=2,I
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          X=AMIN1(DIFC(J),DIFC(J-1))
          TOT=TOT+(TIF(J)-TIF(J-1))*(X+.5*ABS(DIFC(J)-DIFC(J-1)))
   400    CONTINUE
          TTT=TTT+TOT
          WRITE(5,12) TOT
    12    FORMAT(/,"   ***TOTAL CROSS SECTION: ",1PE12.5)
   2000   CONTINUE
          WRITE(5,12) TTT
          STOP
          END

          SUBROUTINE FION(HKE,TEF,DIFCR,TIF,NIST,NHST)
          COMMON/MOM/HKI,SKI,VCM,VI
          COMMON/MASS/HMASS,TMASS,FMASS,RMFH,RMTE,RMTF
          COMMON/CONS/C1,C2,C3,C4,C5,C11,C22,C33,C44,C55
          COMPLEX TD,FF
          DATA ALP,BET,AL1,BE1,AB1,A21,B21,TNC,CONS/1.03323,4.283221,
         *0.639123,-0.713779,0.322451,1.07846,-4.433558,0.035941,1.28E-3/
          DCONS=1.95852E4
          C=137.03602565                            $   CONS=1.6571E-3
          TNC=.025009625
          DCST=0.
          EF=SKI/(2.*RMTH)-1.0+.5*FLOAT(NHST**(-2))+.5*FLOAT(NIST**(-2))
          CEI=COS(TEF)
          CEF=COS(IEF-TIF)
          CIF=COS(TIF)
          SKE=HKE*HKE
          RAD=SKE*CEI*CEI/(TMASS*TMASS)+2.*EF/RMTF-SKE/(RMTF*RMTE)
          HKF=(-HKE*CEI/TMASS+SQRT(RAD))*RMTF
          SKF=HKF*HKF
          SKIF=ABS(SKI+SKF+SKE-2.*HKI*HKF*CIF-2.*HKI*HKE*CEI+2*HKF*HKE*CEF)
          TEK1=C22*SKI+C4+*SKF-2.*C2*C4*CI**HKI*HKF
          TEK2=C22*SKI+SKE-2.*C2*HKE*HKI*CEI
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TER3=C55+SKI+SKE+C33*SKF-2.*C5*HCI
     (CIF+C3.HKF+CEI HKE)+2.*C3*1KE+HKF*CEF
TER4=C55+SKI+SKF-2.*C5 HKI*HKF*CEF
HFI1=F(1,BE1,TER2)*(F(NIST,ALP,TER1)-F(NIST,ALP,TER3))+
   +  F(1,AL1,TER2)*(F(NIST,BET,TER1)-F(NIST,BET,TER3))-
   + F(NIST,ALP,TER4)*F(1,BE1,TER1)-F(NIST,BET,TER4)*F(1,AL1,TER1)
DO 20 NI=1,NHST
N1=NI-1
N2=NHST-N1-1
TD=2*HFI1*(FF(NHST,N1,N2,1.,C44*SKIF)-FF(NHST,N1,N2,1.,C33*SKIF))
  **TNC CONS/SKIF
20 DCST=DCST+CABS(TD)**2
DIFCR=DCST*SKE*SKF*SIN(TEF)*SIN(IIF)*DCONS/(VI SQRT(RAD))
VKF=C*SQRT(1.-(FMASS*C C)**2/((FMASS*C*C)**2+SKF*C*C))
R=VCM/VKF
FACT=(1+R*R+2*R*CIF)**1.5/(1+R*CIF)
DIFCR=DIFCR*FACT
RETURN
END
```

```fortran
      COMPLEX FUNCTION FF(N,N1,N2,A,S)
      COMPLEX TA,YL1,YL2,YK1,YK2,B,C
      IF (S.EQ.0.) GO TO 10
      IF (N.EQ.1) GO TO 20
      BET=.5*SQRT(S)
      ALP=(N*A+1)/(2*N)                $   CONS=A**1.5/(2*N*N)
      GAM=(N*A-1)/(2*N)
      YL1=CMPLX(-ALP,BET)
      YL2=CMPLX(-ALP,-BET)
      YK1=CMPLX(-GAM,BET)
      YK2=CMPLX(-GAM,-BET)
      B=(-(N1+1)*YK1+N1*YL1)*YL2*YK2
      C=(-(N2+1)*YK2+N2*YL2)*YL1*YK1
      TA=YL1**(-N1-2)*YL2**(-N2-2)*YK1**(N1-1)*YK2**(N2-1)
      FF=-CONS*TA*(B+C)
      RETURN
   10 IF(N.EQ.1)  FF=CMPLX(1.,0.)
      RETURN
   20 R=8.*(N+1.)/(((N+1.)**2+S)**2
      FF=CMPLX(R,0.)
      RETURN
      END

      FUNCTION F(N,A,B)
      PI=4*ATAN(1.0)
      IF (N.EQ.2) GO TO 100
      AP=A+1
      F=6*SQRT(PI)*AP/(AP**2+B)**2           $     RETURN
  100 AP=A+.5
      F=8*SQRT(PI/32)*(6*AP**3-3*AP**2+(2*AP+1)*B)/(AP**2+B)**3
      RETURN
      END
```

Vita

Mark Richard Franz was born on 14 April 1956 in Cleveland, Ohio. He graduated from J. W. Nixon High School, Laredo, Texas in June 1974. The next fall he entered Montana State University, Bozeman, Montana graduating in June 1978 with a Bachelor of Science degree in Physics. At that time he received an ROTC commission in the Air Force and was assigned to the Air Force Institute of Technology's resident School of Engineering at Wright-Patterson Air Force Base, Ohio where he earned a Master of Science degree in Engineering Physics.

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The first Born Approximation is used to calculate the differential cross section for electron detachment from H^- ions colliding with Hydrogen atoms. The differential and total cross sections are evaluated for the resultant hydrogen atom in the 1s or 2s state and the target hydrogen atom in any excited state up to $n = 8$. The scattering matrix includes the exchange of particles interaction, which has not been included in earlier work. The results are presented and compared with earlier work where possible.

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